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(54) Title: NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

(57) Abstract

The present invention provides new methods, particularly computational methods, and compositions for the generation of nuclear receptor synthetic ligands based on the three dimensional structure of nuclear receptors, particularly the thyroid receptor (herein referred to as "TR"). Also provided are crystals, nuclear receptor synthetic ligands, and related methods.

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NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

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CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims the benefit of the following provisional applications: 10 United States Ser. No. 60/008,540 and 60/008,543, filed December 13, 1995, and Ser. No. 60/008,606, filed December 14, 1995. This application claims the benefit of the following U.S. patent application: United States Ser. No. 08/764,870, filed December 13, 1996.

INTRODUCTION

Technical Field

This invention relates to computational methods for designing ligands that bind to nuclear receptors, crystals of nuclear receptors, synthetic ligands of nuclear receptors and methods of using synthetic ligands.

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Background

Nuclear receptors represent a superfamily of proteins that specifically bind a physiologically relevant small molecule, such as hormone or vitamin. As a result of a molecule binding to a nuclear receptor, the nuclear receptor changes the ability of a cell to transcribe DNA, i.e. nuclear receptors modulate the transcription of DNA, although they may have transcription independent actions. Unlike integral membrane receptors and membrane associated receptors, the nuclear receptors reside in either the cytoplasm or nucleus of eukaryotic cells. Thus, nuclear receptors comprise a class of intracellular, soluble ligand-regulated transcription factors.

Nuclear receptors include receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so called "orphan receptors" are also

part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors. To date, ligands have not been identified with orphan receptors but it is likely that small molecule ligands will be discovered in the near future for this class of transcription factors. Generally, nuclear receptors specifically bind physiologically relevant small molecules with high affinity and apparent Kd's are commonly in the 0.01 - 20 nM range, depending on the nuclear receptor/ligand pair.

Development of synthetic ligands that specifically bind to nuclear receptors has been largely guided by the trial and error method of drug design despite the importance of nuclear receptors in a myriad of physiological processes and medical conditions such as hypertension, inflammation, hormone dependent cancers (e.g. breast and prostate cancer), modulation of reproductive organ function, hyperthyroidism, hypercholesterolemia and obesity. Previously, new ligands specific for nuclear receptors were discovered in the absence of information on the three dimensional structure of a nuclear receptor with a bound ligand. Before the present invention, researchers were essentially discovering nuclear receptor ligands by probing in the dark and without the ability to visualize how the amino acids of a nuclear receptor held a ligand in its grasp.

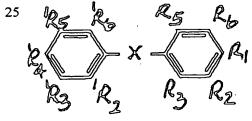
Consequently, it would be advantageous to devise methods and compositions 20 for reducing the time required to discover ligands to nuclear receptors, synthesize such compounds and administer such compounds to organisms to modulate physiological processes regulated by nuclear receptors.

SUMMARY OF THE INVENTION

The present invention provides for crystals of nuclear receptor ligand binding domains with a ligand bound to the ligand binding domain (LBD). The crystals of the present invention provide excellent atomic resolution of the amino acids that interact with nuclear receptor ligand, especially thyroid receptor ligands. The three dimensional model of a nuclear receptor LBD with a ligand bound reveals a previously unknown structure for nuclear receptors and shows that the ligand is bound in a water inaccessible binding cavity of the ligand binding domain of the nuclear receptor.

The present invention also provides for computational methods using three dimensional models of nuclear receptors that are based on crystals of nuclear receptor LBDs. Generally, the computational method of designing a nuclear receptor ligand determines which amino acid or amino acids of a nuclear receptor LBD interact with a chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising a nuclear receptor LBD with a bound ligand, and selecting a chemical modification (at least one) of the chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the corresponding chemical moiety on the natural hormone.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering *in vitro* or *in vivo* a sufficient amount of a compound of the following formula:



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FORMULA I.

where the compound fits specially and preferentially into a nuclear hormone receptor LBD of interest. The method is exemplified by modulating the activity of a thyroid receptor (TR). For modulating TR activity, a compound of Formula I is employed

that fits spacially and preferentially into a TR ligand binding domain (TR LBD), including compounds specific for a TR LBD isoform of interest. Of particular interest are the TR LBD isoforms α (TR-α) and β (TR-β). Additional compounds of interest include derivatives of Formula I, such as those compounds having the biphenyl (φ-X-5) or single phenyl (φ-X or X-φ) nucleus of Formula I and its corresponding substituent groups described herein. Compounds that are interatively designed using structural information gleaned from these compounds and which modulate nuclear hormone receptor activity also are of interest.

The present invention also includes a method for identifying a compound capable of selectively modulating the activity of a nuclear receptor. This aspect of the invention is exemplified by a method for identifying a compound capable of selectively modulating the activity of a TR isoform. The method comprises modeling test compounds that fit spacially and preferentially into a TR LBD isoform of interest using an atomic structural model of a TR LBD isoform bound to a test compound, screening the test compounds in a biological assay for TR isoform activity characterized by binding of a test compound to a TR LBD isoform, and identifying a test compound that selectively modulates the activity of a TR isoform. The compounds may be those of Formula I or derivatives thereof, including compounds having a biphenyl or single phenyl nucleus of Formula I.

Further included is a method for identifying agonist or antagonist ligands of a nuclear receptor using the atomic coordinates of a LBD in conjunction with a computerized modeling system. This aspect of the invention is exemplified by identifying a TR agonist or antagonist ligand by providing the atomic coordinates of a TR LBD to a computerized modeling system, modeling ligands which fit spacially into the TR LBD, and identifying in a biological assay for TR activity a ligand which increases or decreases TR activity. The compounds can be those of Formula I or derivatives thereof, including compounds having a biphenyl or single phenyl nucleus of Formula I.

Also provided is a method of identifying a compound that selectively 30 modulates the activity of one type of nuclear receptor compared to other nuclear hormone receptors. The method is exemplified by modeling test compounds which fit spacially into a TR LBD using an atomic structural model of a TR LBD, selecting a compound comprising conformationally constrained structural features that interact

with conformationally constrained residues of a TR LBD, and identifying in a biological assay for TR activity a compound that selectively binds to a TR LBD compared to other nuclear receptors. The conformationally constrained features involved in receptor-selective ligand binding can be identified by comparing atomic models of receptor isoforms bound to the same and/or different ligands. The methods facilitate design and selection of compounds that have increased selectivity for a particular nuclear receptor. The compounds may be those of Formula I or derivatives thereof, including compounds having the biphenyl or single phenyl nucleus of Formula I.

Another aspect of the invention is a method for increasing the receptor 10 selectivity of a compound for a particular type of nuclear receptor. This involves the chemical modification of a substituent group of a compound of Formula I to generate compounds which have increased selectivity for one type of receptor. For example, chemical modification of a substituent group of the compound of Formula I can be 15 used to introduce additional constraints into a compound that modulates TR activity to increase its selectivity in vivo for TR-type receptors. Additional constraints also may The modified groups will preferably interact with a be added for stability. conformationally constrained structural feature of a TR LBD that is conserved among TR isoforms. A more preferred method comprises selecting compounds having 20 conformationally constrained groups that interact with conformationally constrained residues of a TR LBD conserved among TR isoforms. The compounds can be those of Formula I or derivatives thereof, including compounds having the biphenyl or single phenyl nucleus of Formula I.

The invention finds use in the selection and characterization of peptide,
25 peptidomimetic or synthetic compounds identified by the methods of the invention,
particularly new lead compounds useful in treating disorders related to nuclear
receptor-based deficiencies, including TR-related disorders. For TR-related disorders,
the compounds and methods of the invention can be used to modulate TR activity by
administering to a mammal in need thereof a sufficient amount of compound of
30 Formula I or derivative thereof that fits spacially and preferentially into a TR LBD.

BRIEF DESCRIPTION OF THE DRAWINGS

- FIG. 1 is a diagram illustrating computational methods for designing ligands that interact with nuclear receptors of the nuclear receptor superfamily.
- FIG. 2 is a schematic representation of nuclear receptor structures, indicating 5 regions of homology within family members and functions of the various domains.
 - FIG. 3 shows the aligned amino acid sequences of the ligand binding domains of several members of the nuclear receptor superfamily.
- FIG. 4 is a ribbon drawing of the rat $TR-\alpha$ LBD with secondary structure elements labelled. The ligand (magenta) is depicted as a space-filling model. Alpha 10 helices and coil conformations are yellow, beta strands are blue.
 - FIG. 5 shows two cross-sections of a space-filling model of rat TR- α exposing the ligand (magenta) tightly packed within the receptor.
- FIG. 6 is a schematic of the ligand binding cavity. Residues which interact with the ligand appear approximately at the site of interaction. Hydrogen bonds are shown as dashed lines between the bonding partners; distances for each bond are listed. Non-bonded contacts are shown as radial spokes which face toward interacting atoms.
- FIG. 7 is the distribution of crystallographic temperature factors in the refined rat TR-I LBD. The distribution is represented as a color gradation ranging from less 20 than 15 (dark blue) to greater than 35 (yellow-green).
- FIG. 8 is a ribbon drawing of the rat TR-α LBD showing the c-terminal activation domain to ligand. Residues which comprise the c-terminal activation domain (Pro393-Phe405) are depicted as a stick representation. Hydrophobic residues, particularly Phe401 and Phe405 (blue) face inwards toward the ligand.

 25 Glu403 (red) projects outward into the solvent.
 - FIG. 9 is an electrostatic potential surface of the rat TR-α LBD, calculated using GRAPH. Negative electrostatic potential is red; positive electrostatic potential is blue. The c-terminal activation domain forms a largely hydrophobic (white). The Glu403 is presented as a singular patch of negative charge (red).
- FIG. 10 is a diagram comparing agonists and antagonists for several nuclear receptors.
 - FIG. 11 is the synthetic scheme for preparation of TS1, TS2, TS3, TS4 and TS5.

FIG. 12 is the synthetic scheme for preparation of TS6 and TS7.

- FIG. 13 is the synthetic scheme for preparation of TS8.
- FIG. 14 is the synthetic scheme for preparation of TS10.
- FIG. 15 depicts the chemical structures of several TR ligands.
- 5 FIG. 16 is a graph illustrating competition assays in which T_3 and Triac compete with labeled T_3 for binding to human TR-α or human TR-β.
 - FIG. 17 depicts a Scatchard analysis of labelled T_3 binding to $TR-\alpha$ and $TR-\beta$.
- FIG. 18 is a chart showing the effect of TS-10 on the transcriptional regulation of the DR4-ALP reporter gene in the presence or absence of T3 as assayed 10 in TRAFI1 reporter cells.
 - FIG. 19 is a chart showing the effect of TS-10 on the transcriptional regulation of the DR4-ALP reporter gene in the presence or absence of T3 as assayed in TRAF91 reporter cells.
- FIG. 20 is a chart showing the effect of TS-10 on the transcriptional 15 regulation of the DR4-ALP reporter gene in the presence or absence of T3 as assayed in HepG2, a liver reporter cell line.
 - FIG. 21 is a partial ribbon drawing of TR-α LBD with T3 in the ligand binding cavity. Selected interacting amino acids are labelled, including Ile221, Ile222 and Ser260, Ala263, Ile299 and Leu 276.
- FIG. 22 is a partial ribbon drawing of TR-α LBD with T3 and Dimit superimposed in the ligand binding cavity. Interactions with Ile221, Ile222, Ala260, Ile 299 and Leu276 are labelled.
- FIG. 23 is a partial ribbon drawing of TR-α LBD with T3, illustrating the three Arginine residues (Arg228, Arg262 and Arg 266 (dark stick figures)) of the polar pocket, three water molecules HOH502, HOH503 and HOH504, with hydrogen bonds indicated by dotted lines.
 - FIG. 24 is a partial ribbon drawing of TR- α LBD with Triac, illustrating the three Arginine residues (dark stick figures) of the polar pocket, water molecules (HOH503, HOH504 and HOH600), with hydrogen bonds indicated by dotted lines.
- FIG. 25 is a partial ribbon drawing of the TR-α LBD with T3 and Triac superimposed in the ligand binding cavity. The drawing shows several interacting amino acid residues in the polar pocket that remain unchanged whether T3 or Triac occupies the ligand binding cavity: Arg262, Asn179, HOH503 and HOH504, and

Ser277. Both Arg228 and Arg 266 occupy two different positions, depending on whether T3 or Triac is bound.

- FIG. 26A and 26B are stereochemical representations of the TR- α LBD with Dimit bound.
- 5 FIG. 27 is a partial ribbon drawing of TR-β LBD with GC-1 in the ligand binding cavity. Amino acids Arg282, Arg316, Arg320, Asn 331 and His435 are labelled.
- FIG. 28 is a partial ribbon drawing of TR-β LBD with Triac in the ligand binding cavity. Amino acids Arg282, Arg316, Arg320, Asn331 and His435 are 10 labelled.
 - FIG. 29 is a partial ribbon drawing of TR-βLBD with GC-1 (Blue) overlayed with TR-α LBD with Dimit (Red) in the ligand binding cavities. Amino acids Arg228, Arg262, Arg266 and Ser277 (TR-α LBD), and Arg282, Arg316, Arg320 and Asn331 (TR-β LBD) are labelled.
- FIG. 30 is a partial ribbon drawing of TR-β LBD with Triac (Blue) overlayed with TR-α LBD with Triac (Red) in the ligand binding cavities. Amino acids Arg228, Arg262, Arg266, Ser277 and His381 (TR-α LBD), and Arg282, Arg316, Arg320 and His435 (TR-β LBD) are labelled.
- FIG. 31 is a graph showing competition curves comparing wildtype TR-α and 20 TR-β to a variant TR-β having a single amino acid substitution in the ligand binding domain.
 - FIG. 32 shows atomic numbering for thyronine-like ligands.
 - APPENDIX 1 is an appendix of references.
- APPENDIX 2 is a chart of amino acids that interact with a TR ligand, for TR complexed with Dimit, Triac, IpBr2, T3 and GC-1.
 - APPENDIX 3 is a chart of atomic coordinates for the crystal of rat TR- α LBD complexed with Dimit.
 - APPENDIX 4 is a chart of atomic coordinates for the crystal of rat $TR-\alpha$ LBD complexed with Triac.
- APPENDIX 5 is a chart of atomic coordinates for the crystal of rat TR-α LBD complexed with IpBr₂.

APPENDIX 6 is a chart of atomic coordinates for the crystal of rat $TR-\alpha$ LBD complexed with T_3 .

APPENDIX 7 is a chart of atomic coordinates for the crystal of human TR- β LBD complexed with Triac.

5 APPENDIX 8 is a chart of atomic coordinates for the crystal of human TR-β-LBD complexed with GC-1.

DETAILED DESCRIPTION OF THE INVENTION

Introduction

The present invention provides new methods, particularly computational methods, and compositions for the generation of nuclear receptor synthetic ligands based on the three dimensional structure of nuclear receptors, particularly the thyroid receptor (herein referred to as "TR"). Previously, the lack of three dimensional structural information about the ligand binding domain of a nuclear receptor thwarted the field of nuclear receptor drug discovery, especially the absence of three dimensional structural information relating to a nuclear receptor with a ligand bound.

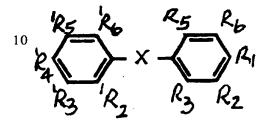
Described herein for the first time are crystals and three dimensional structural information from a nuclear receptor's ligand binding domain (LBD) with a ligand bound. The structure of the TR LBD complexed with 3,5,3'-triiodothyronine (T₃), 20 3,5-dibromo-3'-isopropylthyronine (IpBr₂), 3,5- dimethyl-3'-isopropylthyronine (Dimit), and 3,5,3'-triiodothyroacetic acid (Triac), 3,5-dimethyl-4-(4'-hydroxy-3'isopropylbenzyl)-phenoxy acetic acid (GC1) are exemplified. Such crystals offer superior resolution at the atomic level and the ability to visualize the coordination of nuclear receptor ligands by amino acids that comprise the LBD. The present 25 invention also provides computational methods for designing nuclear receptor synthetic ligands using such crystal and three dimensional structural information to generate synthetic ligands that modulate the conformational changes of a nuclear receptor's LBD. Such synthetic ligands can be designed using the computational methods described herein and shown, in part, in FIG. 1. These computational 30 methods are particularly useful in designing an antagonist or partial agonist to a nuclear receptor, wherein the antagonist or partial agonist has an extended moiety that prevents any one of a number of ligand-induced molecular events that alter the receptor's influence on the regulation of gene expression, such as preventing the

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normal coordination of the activation domain observed for a naturally occurring ligand or other ligands that mimic the naturally occurring ligand, such as an agonist. As described herein, synthetic ligands of nuclear receptors will be useful in modulating nuclear receptor activity in a variety of medical conditions.

Of particular interest is use of such ligands in a method of modulating TR activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound of Formula I,



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where the compound fits spatially and preferentially into a TR LBD. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a TR LBD. By "TR LBD" is intended a structural segment or segments of thyroid hormone receptor polypeptide 20 chain folded in such a way so as to give the proper geometry and amino acid residue configuration for ligand binding. This is the physical arrangement of protein atoms in three-dimensional space forming a ligand binding pocket or cavity. By "fits spacially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a TR LBD. Compounds of 25 interest also include derivatives of Formula I. By "derivatives of Formula I" is intended compounds that comprise at least a single phenyl scaffold (\$\phi\$-X or X-\$\phi\$) of the biphenyl scaffold (ϕ -X- ϕ) of Formula I which comprise the corresponding substituents of Formula I described herein. Compounds that are interatively designed using structural information gleaned from these compounds and which 30 modulate nuclear hormone receptor activity also are of interest. Preferred compounds of Formula I and its derivatives that fit spacially and preferentially into a TR LBD comprise the following substituents:

(i) an R1-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue from the group Arg228, Arg262, and Arg266 of human TR-α, and Arg282, Arg316 and Arg320 of human TR-β, where the anionic group is about 1.7-4.0Å from the nitrogen atom;

- 5 (ii) an R2-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- (iii) an R3-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a serine, alanine and/or isoleucine corresponding to a residue from the group Ser260, Ala263 and Ile299 of human TR-α, and Ser314,
 10 Ala317 and Ile352 of human TR-β, where the hydrophobic or hydrophilic group is about 1.7-4.0Å from the side chain atom;
- (iv) an R5-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a phenylalanine and/or isoleucine corresponding to a residue from the group Phe218, Ile221 and Ile222 of human TR-α, and Phe272,
 15 Ile275 and Ile276 of human TR-β, where the hydrophobic or hydrophilic group is about 1.7-4.0Å from the side chain atom;
 - (v) an R6-substitutent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- (vi) an X-substituent comprising a hydrophobic or hydrophilic group that 20 interacts with a side chain atom of a leucine corresponding to a residue from the group Leu276 and Leu292 of human TR-α, and Leu 330 and Leu346 of human TR-β, where the hydrophobic or hydrophilic group is about 1.7-4.0Å from the side chain atom;
- (vii) an R2'-substituent comprising a hydrophobic or hydrophilic group that 25 fits spacially into the TR LBD;
- (viii) an R3'-substituent comprising a hydrophobic group that interacts with a side chain atom of a phenylalanine, glycine and/or methionine corresponding to a residue from the group Phe215, Gly290, and Met388 of human TR-α, and Phe269, Gly344, Met442 of human TR-β, where the hydrophobic group is about 1.7-4.0Å 30 from the side chain atom:
 - (ix) an R4'-substituent comprising an hydrogen bond donor or acceptor group that interacts with a side chain carbon or nitrogen atom of a histidine corresponding to residue His381 of human $TR-\alpha$, and His435 of human $TR-\beta$, where

the hydrogen bond donor or acceptor group is about 1.7-4.0Å from the side chain atom;

- (x) an R5'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- 5 (xi) and R6'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD; and

where the compound is other than thyronine (T3), triiodothyronine (T4) or other thyronine-like compounds previously known and used in a TR treatment method, such as those referenced in Appendix I.

10 Examples of such substituents include the following: where R_1 is

-CH₂CH[NH-tBOC]CO₂H, or a carboxylate connected to the ring with a 0 to 3 carbon linker,

phosphonate connected to the ring with a 0 to 3 carbon linker,

-PO₃H₂, -CH₂PO₃H₂, -CH₂CH₂PO₃H₂, -CH₂CHNH₂PO₃H₂, -CH₂CH[NHCOCH ϕ_2]PO₃H₂, -CH₂CH[NHCO(CH₂)₁₅CH₃]PO₃H₂, -CH₂CH[NH-FMOC]PO₃H₂, -CH₂ CH[NH-tBOC]PO₃H₂, or a phosphate or

-SO₃H, -CH₂SO₃H, -CH₂CH₂SO₃H, -CH₂CH[NHCOCH ϕ_2]SO₃H, -CH₂CH[NHCO(CH₂)₁₅CH₃]SO₃H,

-CH₂CH[NH-FMOC]SO₃H, -CH₂ CH[NH-tBOC]SO₃H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon linker, or acts as the functional

equivalent of CH₂CH(NH₂)CO₂H of T3 in the molecular recognition domain when bound to a TR, wherein R₁ can be optionally substituted with an amine, where R₂ is

H, halogen, CF₃, OH, NH₂, SH, CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

30 where R₃ is

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-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR, where R_5 is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR, and R_3 can be identical to R_5 ,

where R₆ is

5 -H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR, and R₂ can be identical to R₆,

where R2' is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

where R₃' is any hydrophobic group, including

halogen, -CF₃, -SH, alkyl, aryl, 5- or 6-membered heterocyclie, cyano, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

15 where R₄' is

-H, halogen, -CF₃, -OH, -NH₂, NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, -SH, -CH₃, -Et, or akyl, aryl or 5- or 6-membered heterocyclic aromatic attached through urea or carbamate linkages to O or N or S at the R₄' position, or acts as the functional equivalent of OH in the molecular recognition domain when bound to a TR,

where R₅' is

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-H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups,

where R₆' is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

where X is

O, S, SO₂, NH, NR₇, CH₂, CHR₇, CR₇R₇, wherein R₇ is alkyl, aryl or 5- or 6-membered heterocyclic aromatic,

and where the TR LBD ligand has an apparent Kd for binding TR LBD of 1 TM or 5 less.

Of particular interest are the class of compounds according to Formula I having the following substituents: where R₁ is carboxylate, phosphonate, phosphate or sulfite and is connected to the ring with a 0 to 3 carbon linker, R₂ is H, R₃ is -I, -Br, or -CH₃, R₅ is -I, -Br, or -CH₃, R₆ is H, R₂' is H, R₃' is -I, -Br, -CH₃, -iPr, -phenyl, 10 benzyl, or 5- or 6-membered ring heterocycles, R₄' is -OH, -NH₂, and -SH, R₅' is -H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, 15 aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups, and R₆' is H.

The present invention also includes a method for identifying a compound 20 capable of selectively modulating the activity of a TR isoform. By "modulating" is intended increasing or decreasing activity of a TR. By "TR isoform" is intended TR proteins encoded by subtype and variant TR genes. This includes TR-α and TR-β isoforms encoded by different genes (e.g., thra and thrb) and variants of the same 25 genes (e.g., thrb1 and thrb2). The method comprises the steps of modeling test compounds that fit spacially and preferentially into a TR LBD isoform of interest using an atomic structural model of a TR LBD isoform bound to a test compound, screening the test compounds in a biological assay for TR isoform activity characterized by binding of a test compound to a TR LBD isoform, and identifying a 30 test compound that selectively modulates the activity of a TR isoform. "modeling" is intended quantitative and qualitative analysis of receptor-ligand structure/function based on three-dimensional structural information and receptor-This includes conventional numeric-based molecular ligand interaction models.

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dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods.

For selectively modulating activity of a TR isoform, such as TR-α or TR-β, a sufficient amount of a compound that fits spatially and preferentially into TR LBD isoform is provided *in vitro* or *in vivo* to achieve the desired end result. TR-α isoform selectivity can be accomplished with a compound comprising an anionic group that interacts with an oxygen or carbon of a serine residue corresponding to Ser277 of human TR-α, where the anionic group is about 1.7-4.0Å from the side chain atom. TR-β isoform selectivity can be accomplished with a compound comprising an anionic group that interacts with the side chain nitrogen of an asparagine corresponding to Asn331 of human TR-β, where the anionic group is about 1.7-4.0Å from the side chain nitrogen atom.

The present invention further includes a method for identifying a TR agonist or antagonist ligand by providing the atomic coordinates of a TR LBD to a computerized modeling system, modeling ligands which fit spacially into the TR LBD, and identifying in a biological assay for TR activity a ligand which increases or decreases the activity of the TR.

The invention also involves a method for increasing receptor selectivity of a compound of Formula I or derivatives thereof for a TR-type receptor versus other nuclear receptors by selecting a compound that interacts with conformationally constrained residues of a TR LBD that are conserved among TR isoforms. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. In designing and selecting compounds having increased specificity for TRs compared to other nuclear receptors, the following methods of the invention can be used. One method involves comparing atomic models of a first TR LBD isoform bound to a compound with a second TR LBD isoform bound to the same compound, identifying atoms of the TR LBD and compounds which interact, and designing or selecting a compound that interacts with TR LBD residues comprising a conformationally constrained structural feature that is conserved between the TR LBD isoforms. Another method relates to comparing a

first TR LBD complexed with a first compound to a second TR LBD complexed with a second compound having one or more different substituents compared to the first compound, identifying atoms of the TR LBD and compounds which interact, and designing or selecting compounds that interact with TR LBD residues comprising a 5 conformationally constrained structural feature that is conserved between the TR LBD isoforms. The methods also facilitate identification of structural and conformationally constrained interactions that are conserved between compounds that bind to a TR LBD. The methods are exemplified by comparing atomic models of a first TR LBD isoform complexed with a first compound of Formula I to a second TR LBD isoform 10 complexed with the first compound, or a second compound of Formula I having different substituents than the first compound. For example, a TR- α LBD bound to a natural hormone such as T3 is compared to a TR-β LBD bound to an organic thyronine-like compound such as GC-1. Conserved contacts are identified which are made between atoms of the different compounds and atoms of the TR LBDs, and the 15 fiducial and adjustable components identified. Compounds selective for TR are identified in a biological assay for TR activity that assays for selective binding to a TR and/or TR LBD compared to other nuclear receptors. Conventional assays for TR and other nuclear receptors may be conducted in parallel or serially, including those assays described herein. Automatable methods are preferred. The methods facilitate 20 design and selection of compounds comprising cyclic carbon and substituent atoms that interact with a constrained side chain and/or main chain atom of a TR LBD residue.

In another aspect of the invention, the methods described herein are useful for selecting peptides, peptidomimetics or synthetic molecules that modulate TR activity.

25 Methods of the invention also find use in characterizing structure/function relationships of natural and synthetic TR-ligands. Molecules of particular interest are new thyronine-like compounds other than T3, T4 and other thyronine-like compounds previously known and used for treating TR-related disorders. New compounds of the invention include those which bind to a TR LBD isoform with greater affinity than T3 or T4 and those which exhibit isoform-specific binding affinity.

APPLICABILITY TO NUCLEAR RECEPTORS

The present invention, particularly the computational methods, can be used to design drugs for a variety of nuclear receptors, such as receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens 5 (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoid (RARs and RXRs), icosanoid (IRs), and peroxisomes (XPARS and peroxisomal proliferators (PPAP)). The present invention can also be applied to the "orphan receptors," as they are structurally homologous in terms of modular domains and primary structure to classic nuclear receptors, such as steroid and thyroid receptors. The amino acid homologies 10 of orphan receptors with other nuclear receptors ranges from very low (<15%) to in the range of 35% when compared to rat RARI and human TR-β receptors, for example. In addition, as is revealed by the X-ray crystallographic structure of the TR and structural analysis disclosed herein, the overall folding of liganded superfamily members is likely to be similar. Although ligands have not been identified with 15 orphan receptors, once such ligands are identified one skilled in the art will be able to apply the present invention to the design and use of such ligands, as their overall structural modular motif will be similar to other nuclear receptors described herein.

Modular Functional Domains Of Nuclear receptors

- The present invention will usually be applicable to all nuclear receptors, as discussed herein, in part, to the patterns of nuclear receptor activation, structure and modulation that have emerged as a consequence of determining the three dimensional structures of nuclear receptors with different ligands bound, notably the three dimensional structures or crystallized protein structure of the ligand binding domains 25 for TR-α and TR-β. Proteins of the nuclear receptor superfamily display substantial regions of amino acid homology, as described herein and known in the art see FIG. 2. Members of this family display an overall structural motif of three modular domains (which is similar to the TR three modular domain motif):
 - 1) a variable amino-terminal domain;

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- 2) a highly conserved DNA-binding domain (DBD); and
 - 3) a less conserved carboxyl-terminal LBD.

The modularity of this superfamily permits different domains of each protein to separately accomplish different functions, although the domains can influence each

other. The separate function of a domain is usually preserved when a particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques a modular domain can sometimes be separated from the parent protein. Using conventional molecular biology techniques each domain can usually be separately expressed with its original function intact or chimerics of two different nuclear receptors can be constructed, wherein the chimerics retain the properties of the individual functional domains of the respective nuclear receptors from which the chimerics were generated.

FIG. 2 provides a schematic representation of family member structures, 10 indicating regions of homology within family members and functions of the various domains.

Amino Terminal Domain

The amino terminal domain is the least conserved of the three domains and varies markedly in size among nuclear receptor superfamily members. For example, this domain contains 24 amino acids in the VDR and 603 amino acids in the MR. This domain is involved in transcriptional activation and in some cases its uniqueness may dictate selective receptor-DNA binding and activation of target genes by specific receptor isoforms. This domain can display synergistic and antagonistic interactions with the domains of the LBD. For example, studies with mutated and/or deleted receptors show positive cooperativity of the amino and carboxy terminal domains. In some cases, deletion of either of these domains will abolish the receptor's transcriptional activation functions.

25 DNA-Binding Domain

The DBD is the most conserved structure in the nuclear receptor superfamily. It usually contains about 70 amino acids that fold into two zinc finger motifs, wherein a zinc ion coordinates four cysteines. DBDs contain two perpendicularly oriented I-helixes that extend from the base of the first and second zinc fingers. The two zinc 30 fingers function in concert along with non-zinc finger residues to direct nuclear receptors to specific target sites on DNA and to align receptor homodimer or heterodimer interfaces. Various amino acids in DBD influence spacing between two half-sites (usually comprised of six nucleotides) for receptor dimer binding. For

example, GR subfamily and ER homodimers bind to half-sites spaced by three nucleotides and oriented as palindromes. The optimal spacings facilitate cooperative interactions between DBDs, and D box residues are part of the dimerization interface. Other regions of the DBD facilitate DNA-protein and protein-protein interactions required for RXR homodimerization and heterodimerization on direct repeat elements.

The LBD may influence the DNA binding of the DBD, and the influence can also be regulated by ligand binding. For example, TR ligand binding influences the degree to which a TR binds to DNA as a monomer or dimer. Such dimerization also depends on the spacing and orientation of the DNA half sites. The receptors also can interact with other proteins and function to regulate gene expression.

The nuclear receptor superfamily has been subdivided into two subfamilies: 1) GR (GR, AR, MR and PR) and 2) TR (TR, VDR, RAR, RXR, and most orphan receptors) on the basis of DBD structures, interactions with heat shock proteins (hsp), and ability to form heterodimers. GR subgroup members are tightly bound by hsp in the absence of ligand, dimerize following ligand binding and dissociation of hsp, and show homology in the DNA half sites to which they bind. These half sites also tend to be arranged as palindromes. TR subgroup members tend to be bound to DNA or other chromatin molecules when unliganded, can bind to DNA as monomers and dimers, but tend to form heterodimers, and bind DNA elements with a variety of orientations and spacings of the half sites, and also show homology with respect to the nucleotide sequences of the half sites. By this classification, ER does not belong to either subfamily, since it resembles the GR subfamily in hsp interactions, and the TR subfamily in nuclear localization and DNA-binding properties.

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Ligand Binding Domain

The LBD is the second most highly conserved domain in these receptors. Whereas integrity of several different LBD sub-domains is important for ligand binding, truncated molecules containing only the LBD retain normal ligand-binding activity. This domain also participates in other functions, including dimerization, nuclear translocation and transcriptional activation, as described herein. Importantly, this domain binds the ligand and undergoes ligand-induced conformational changes as detailed herein.

Most members of the superfamily, including orphan receptors, possess at least two transcription activation subdomains, one of which is constitutive and resides in the amino terminal domain (AF-1), and the other of which (AF-2 (also referenced as TAU 4)) resides in the ligand-binding domain whose activity is regulated by binding of an agonist ligand. The function of AF-2 requires an activation domain (also called transactivation domain) that is highly conserved among the receptor superfamily (approximately amino acids 1005 to 1022). Most LBDs contain an activation domain. Some mutations in this domain abolish AF-2 function, but leave ligand binding and other functions unaffected. Ligand binding allows the activation domain to serve as an interaction site for essential co-activator proteins that function to stimulate (or in some cases, inhibit) transcription.

For example, Shibata, H., et al. (Recent Progress in Hormone Res. 52:141-164 (1997)) has reviewed the role of co-activators and co-repressors in steroid/thyroid hormone receptor systems. Steroid receptor co-activator-one (SRC-1) appears to be a 15 general co-activator for all AF-2 domain containing receptors tested. SRC-1 enhances transactivation of steroid hormone-dependent target genes. Other putative coactivators have been reported, including the SRC-1 related proteins, TIF-2 and GRIP-1, and other putative unrelated co-activators such as ARA-70, Trip 1, RIP-140, and TIF-1. In addition another co-activator CREB-binding protein (CBP) has been shown 20 to enhance receptor-dependent target gene transcription. CBP and SRC-1 interact and synergistically enhance trancriptional activation by the ER and PR. A ternary complex of CBP, SRC-1, and liganded receptors-may form to increase the rate of hormone-responsive gene transcription. Co-repressors, such as SMRT and N-CoR, for TR and RAR, have been identified that also contribute to the silencing function of 25 unliganded TR. The unliganded TR and RAR have been shown to inhibit basal promoter activity; this silencing of target gene transcription by unliganded receptors is mediated by these co-repressors. The collective data suggests that upon binding of agonist, the receptor changes its conformation in the ligand-binding domain that enables recruitment of co-activators, which allows the receptor to interact with the 30 basal transcriptional machinery more efficiently and to activate transcription. contrast, binding of antagonists induces a different conformational change in the receptor. Although some antagonist-bound receptors can dimerize and bind to their cognate DNA elements, they fail to dislodge the associated co-repressors, which results in a nonproductive interaction with the basal transcriptional machinery.

Similarly, the TR and RAR associate with co-repressors in the absence of ligand, thereby resulting in a negative interaction with the transcriptional machinery that silences target gene expression. In the case of mixed agonist/antagonists, such as 4-hydroxytamoxifen, activation of gene transcription may depend on the relative ratio of co-activators and co-repressors in the cell or cell-specific factors that determine the relative agonistic or antagonistic potential of different compounds. These co-activators and co-repressors appear to act as an accelerator and/or a brake that modulates transcriptional regulation of hormone-responsive target gene expression.

The carboxy-terminal activation subdomain, as described herein is in close three dimensional proximity in the LBD to the ligand, so as to allow for ligands bound to the LBD to coordinate (or interact) with amino acid(s) in the activation subdomain. As described herein, the LBD of a nuclear receptor can be expressed, crystallized, its three dimensional structure determined with a ligand bound (either using crystal data from the same receptor or a different receptor or a combination thereof), and computational methods used to design ligands to its LBD, including ligands that contain an extension moiety that coordinates the activation domain of the nuclear receptor.

Once a computationally designed ligand (CDL) is synthesized as described herein and known in the art, it can be tested using assays to establish its activity as an 20 agonist, partial agonist or antagonist, and affinity, as described herein. After such testing, the CDLs can be further refined by generating LBD crystals with a CDL bound to the LBD. The structure of the CDL can then be further refined using the chemical modification methods described herein for three dimensional models to improve the activity or affinity of the CDL and make second generation CDLs with 25 improved properties, such as that of a super agonist or antagonist described herein. Agonist and antagonist ligands also can be selected that modulate nuclear receptor responsive gene transcription through altering the interaction of co-activators and corepressors with their cognate nuclear hormone receptor. For example, CDL agonists can be selected that block or dissociate the co-repressor from interaction with the 30 receptor, and/or which promote binding or association of the co-activator. CDL antagonists can be selected that block co-activator interaction and/or promote corepressor interaction with the target receptor. Selection can be done in binding assays that screen for CDLs having the desired agonist or antagonist properties. Suitable assays for such screening are described herein and in Shibata, H., et al. (Recent Prog.

Horm. Res. 52:141-164 (1997)); Tagami, T., et al. (Mol. Cell Biol. 17(5):2642-2648 (1997)); Zhu, XG., et al. (J. Biol. Chem. 272(14):9048-9054 (1997)); Lin, B.C., et al. (Mol. Cell Biol. 17(10):6131-6138 (1997)); Kakizawa, T., et al. (J. Biol. Chem. 272(38):23799-23804 (1997)); and Chang, K. H., et al. (Proc. Natl. Acad. Sci. USA 94(17):9040-9045 (1997)), which references are incorporated herein in their entirety by reference.

NUCLEAR RECEPTOR ISOFORMS

The present invention also is applicable to generating new synthetic ligands to distinguish nuclear receptor isoforms. As described herein, CDLs can be generated that distinguish between binding isoforms, thereby allowing the generation of either tissue specific or function specific synthetic ligands. For instance, GR subfamily members have usually one receptor encoded by a single gene, although are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α, β) or three (RAR, RXR, and PPAR: α, β, γ) genes or have alternate RNA splicing and such an example for TR is described herein.

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NUCLEAR RECEPTOR CRYSTALS

The invention provides for crystals made from nuclear receptor ligand binding domains with the ligand bound to the receptor. As exemplified in the Examples, TRs are crystallized with a ligand bound to it. Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (co-crystals) for the same nuclear receptor are separately made using different ligands, such as a naturally occurring ligand and at least one bromo- or iodosubstituted synthetic ligand that acts as an analog or antagonist of the naturally occurring ligand. Such bromo- and iodo- substitutions act as heavy atom substitutions in nuclear receptor ligands and crystals of nuclear receptor proteins. This method has the advantage for phasing of the crystal in that it bypasses the need for obtaining traditional heavy metal derivatives. After the three dimensional structure is determined for the nuclear receptor LBD with its ligand bound, the three dimensional

structure can be used in computational methods to design a synthetic ligand for the nuclear receptor and further activity structure relationships can be determined through routine testing using the assays described herein and known in the art.

5 Expression and Purification of other Nuclear Receptor LBD Structures

High level expression of nuclear receptor LBDs can be obtained by the techniques described herein as well as others described in the literature. High level expression in E. coli of ligand binding domains of TR and other nuclear receptors, including members of the steroid/thyroid receptor superfamily, such as the receptors 10 ER, AR, MR, PR, RAR, RXR and VDR can also be achieved. Yeast and other eukaryotic expression systems can be used with nuclear receptors that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human 15 RAR-α, human RAR-γ, human RXR-α, human RXR-β, human PPAR-α, human PPAR-β, human PPAR-γ, human VDR, human ER (as described in Seielstad et al., Molecular Endocrinology, vol 9:647-658 (1995), incorporated herein by reference), human GR, human PR, human MR, and human AR. The ligand binding domain of each of these nuclear receptors has been identified and is shown in FIG. 3. Using the 20 information in FIG. 3 in conjunction with the methods described herein and known in the art, one of ordinary skill in the art could express and purify LBDs of any of the nuclear receptors, including those illustrated in FIG. 3, bind it to an appropriate ligand, and crystallize the nuclear receptor's LBD with a bound ligand.

FIG. 3 is an alignment of several members of the steroid/thyroid hormone 25 receptor superfamily that indicates the amino acids to be included in a suitable expression vector.

Extracts of expressing cells are a suitable source of receptor for purification and preparation of crystals of the chosen receptor. To obtain such expression, a vector is constructed in a manner similar to that employed for expression of the rat TR 30 alpha (Apriletti et al. Protein Expression and Purification, 6:363-370 (1995), herein incorporated by reference). The nucleotides encoding the amino acids encompassing the ligand binding domain of the receptor to be expressed, for example the estrogen receptor ligand binding domain (hER-LBD) (corresponding to R at position 725 to L

at position 1025 as standardly aligned as shown in the FIG. 3), are inserted into an expression vector such as the one employed by Apriletti et al (1995). For the purposes of obtaining material that will yield good crystals it is preferable to include at least the amino acids corresponding to human TR-β positions 725 to 1025.

5 Stretches of adjacent amino acid sequences may be included if more structural information is desired. Thus, an expression vector for the human estrogen receptor can be made by inserting nucleotides encoding amino acids from position 700 to the c-terminus at position 1071. Such a vector gives high yield of receptor in E. coli that can bind hormone (Seielstad et al. Molecular Endocrinology 9:647-658 (1995)).

10 However, the c-terminal region beyond position 1025 is subject to variable proteolysis and can advantageously be excluded from the construct, this technique of avoiding variable proteolysis can also be applied to other nuclear receptors.

TR-α And TR-β As Examples of Nuclear receptor LBD Structure and Function 15 TR Expression, Purification And Crystallization

As an example of nuclear receptor structure of the ligand binding domain the α- and β- isoforms of TR are crystallized from proteins expressed from expression constructs, preferably constructs that can be expressed in E. coli. Other expression systems, such as yeast or other eukaryotic expression systems can be used. For the 20 TR, the LBD can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR-α, Glu 202 to Asp 461 of the human TR-β.

Typically TR LBDs are purified to homogeneity for crystallization. Purity of TR LBDs is measured with sodium dodecyl sulfate polyacrylamide gel 30 electrophoresis (SDS-PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified TR for crystallization should be at least 97.5 % pure or 97.5%, preferably at least 99.0% pure or 99.0% pure, more preferably at least 99.5% pure.

Initially purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

To achieve higher purification for improved crystals of nuclear receptors, 5 especially the TR subfamily and TR, it will be desirable to ligand shift purify the nuclear receptor using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, 10 the receptor then elutes at the position of the liganded receptor are removed by the original column run with the unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

More recently developed methods involve engineering a "tag" such as with histidine placed on the end of the protein, such as on the amino terminus, and then using a nickle chelation column for purification, Janknecht R., *Proc. Natl. Acad. Sci. USA*, 88:8972-8976 (1991) incorporated by reference.

20 To determine the three dimensional structure of a TR LBD, or a LBD from another member of the nuclear receptor superfamily, it is desirable to co-crystalize the LBD with a corresponding LBD ligand. In the case of TR LBD, it is preferable to separately co-crystalize it with ligands such as T3, IpBr and Dimit that differ in the heavy atoms which they contain. Other TR ligands such as those encompassed by 25 Formula 1 described herein and known in the prior art, can also be used for the generation of co-crystals of TR LBD and TR ligands. Of the compounds encompassed by Formula 1 it is generally desirable to use at least one ligand that has at least one bromo- or iodo- substitution at the R₃, R₅, R₃' or R₅' position, preferably such compounds will be have at least two such substitutions and more preferably at 30 least 3 such substitutions. As described herein, such substitutions are advantageously used as heavy atoms to help solve the phase problem for the three dimensional structure of the TR LBD and can be used as a generalized method of phasing using a halogen (e.g. I or Br) substituted ligand, especially for nuclear receptors.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range.

Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. In the case of TR it is preferable to use crystallization temperatures from 18 to 25°C, more preferably 20 to 23°C, and most preferably 22°C.

Complexes of the TR-\alpha LBD with a variety of agonists, including T₃, IpBr₂, Dimit, and Triac, are prepared with by methods described herein. For example, cocrystals of the rTR-α LBD, with ligand prebound, are prepared by vapor diffusion at ambient temperature from 15% 2-methyl-2,4-pentanediol (MPD). The crystals are 15 radiation sensitive, and require freezing to measure complete diffraction data. On a rotating anode X-ray source, the crystals diffract to ~3Å; synchrotron radiation extends the resolution limit significantly, to as high as 2.0Å for T₃ cocrystals. The composition of the thyroid hormone, combined with the ability to prepare and cocrystallize the receptor complexed with a variety of analogs, permitted the unusual 20 phasing strategy. This phasing strategy can be applied to the ligands of the nuclear receptors described therein by generating I and Br substitutions of such ligands. In this strategy, cocrystals of the TR LBD containing four hormone analogs that differ at the 3,5, and 3' positions (T₃, IpBr₂, Dimit, and Triac) provided isomorphous derivatives. For this set of analogs, the halogen substituents (2Br and 3I atoms) 25 function as heavy atoms, while the Dimit cocrystal (3 alkyl groups) acts as the parent. The initial 2.5Å multiple isomorphous replacement/anomalous scattering/density modified electron density map allowed the LBD to be traced from skeletons created in the molecular graphics program O5 (Jones, T.A. et al., ACTA Cryst, 47:110-119 (1991), incorporated by reference herein). A model of the LBD was built in four 30 fragments, Arg157-Gly184, Trp186-Gly197, Ser199-Pro205, and Val210-Phe405, and refined in XPLOR using positional refinement and simulated annealing protocols. Missing residues were built with the aid of difference density. The final model was refined to $R_{cryst} = 21.8\%$ and $R_{free} = 24.4\%$ for data from 15.0 to 2.2Å, see Table 6.

The human TR- β LBD model was resolved by molecular replacement of the TR- α LBD coordinates. The structure is based on E202 to D461 with a his-tag at the N-terminus. The final model was refined to R_{cryst} = 25.3% and R_{free} = 28.9% for data from 30.0 to 2.4Å+, see Table 7.

This phasing strategy can be applied to the ligands of the nuclear receptors described herein by generating I and Br substitutions of such ligands.

THREE DIMENSIONAL STRUCTURE OF TR LBD Architecture of TR LBD

As an example of the three dimensional structure of a nuclear receptor, the folding of the TR-α LBD is shown in FIG. 4. The TR-α LBD consists of a single structural domain packed in three layers, composed of twelve α-helices, H1-12, and four short β-strands, S1-4, forming a mixed β-sheet. The buried hormone and three antiparallel α-helices, H5-6, H9, and H10, form the central layer of the domain, as 15 shown in FIG. 4. H1, H2, H3 and S1 form one face of the LBD, with the opposite face formed by H7, H8, H11, and H12. The first 35 amino acids of the N-terminus (Met122-Gln156) are not visible in the electron density maps. The three dimensional structure of the heterodimeric RXR:TR DNA-binding domains bound to DNA, amino acids Met 122 - Gln151 of the TR DBD make extensive contacts with the minor 20 groove of the DNA8. The five disordered amino acids (Arg152-Gln156), which reside between the last visible residue of the TR DBD and the first visible residue of the LBD likely represent the effective "hinge" linking the LBD and the DBD in the intact receptor.

The predominantly helical composition and the layered arrangement of 25 secondary structure is identical to that of the unliganded hRXR α , confirming the existence of a common nuclear receptor fold between two nuclear receptors.

The TR LBD is visible beginning at Arg157, and continues in an extended coil conformation to the start of H1. A turn of α-helix, H2, covers the hormone binding cavity, immediately followed by short β-strand, S1, which forms the edge of the 30 mixed β-sheet, parallel to S4, the outermost of the three antiparallel strands. The chain is mostly irregular until H3 begins, antiparallel to H1. H3 bends at Ile221 and Ile222, residues which contact the ligand. The chain turns almost 90° at the end of H3 to form an incomplete α-helix, H4. The first buried core helix, H5-6, follows, its axis

altered by a kink near the ligand at Gly 253. The helix is composed of mostly hydrophobic sidechains interrupted by two striking exceptions: Arg262 is solvent inaccessible and interacts with the ligand carboxylate (1-substituent), and Glu256 meets Arg329 from H9 and Arg375 from H11 in a polar invagination. 5 terminates in a short β-strand, S2, of the four strand mixed sheet. S3 and S4 are joined through a left-handed turn, and further linked by a salt bridge between Lys284 and Asp272. Following S4, H7 and H8 form an L, stabilized by a salt bridge between Lys268 and Asp277. The turn between H7 and H8 adopts an unusual conformation, a result of interaction with ligand and its glycine rich sequence. H9 is the second core 10 helix. antiparallel to the neighboring H5-6. Again, two buried polar sidechains are found, Glu315 and Gln320. Glu315 forms a buried salt bridge with His358 and Arg356. The oxygen of Gln320 forms a hydrogen bond with the buried sidechain of His 175. The chain then switches back again to form H10, also antiparallel to H9. H11 extends diagonally across the full length of the molecule. Immediately after H11, the 15 chain forms a type II turn, at approximately 90° to H11. The chain then turns again to form H 12, which packs loosely against H3 and H11 as part of the hormone or ligand binding cavity. The final five amino acids at the C-terminus, Glu406 -Val410, are disordered. The architecture of the TR- β LBD is identical to that of the TR- α LBD, with two significant differences. An additional helix is present at the N-terminus 20 (residues Glu202-I1e208), which is part of the DBD, and packs antiparallel to H10. Following the helix is a two residue turn (Gly209-His210) continuing into an extended coil to he start of H1, as seen in the TR-α LBD. A further difference occurs in the irregular conformation adopted between H2 and H3. In the TR-\alpha LBD, residue Gly197-Asp211 form a loop that packs against the receptor, contacting helices H7, 25 H8, H11, and the loop between H11 and H12. In the TR-β LBD, only the ends of the loop are ordered, with the stretch Ala253-Lys263 disordered. In addition to these residues, the residues of the His-tag at the N-terminus, and the final residue at the Cterminus, Asp461, are disordered.

30 TR LBD's Ligand Binding Cavity As An Example Of A Nuclear Receptor's Buried Ligand Cavity

The three dimensional structure of the TR LBD leads to the startling finding that ligand binding cavity of the LBD is solvent inaccessible when a T3 or its isostere

is bound to the LBD. This surprising result leads to a new model of nuclear receptor three dimensional structure and function, as further described herein, particularly in the sections elucidating the computational methods of ligand design and the application of such methods to designing nuclear receptor synthetic ligands that 5 contain extended positions that prevent normal activation of the activation domain.

Dimit, the ligand bound to the receptor, is an isostere of T₃ and a thyroid hormone agonist. Therefore the binding of Dimit should reflect that of T₃, and the Dimit-bound receptor is expected to be the active conformation of TR. The ligand is buried within the receptor, providing the hydrophobic core for a subdomain of the 10 protein, as shown in FIG. 5 a and b. H5-6 and H9 comprise the hydrophobic core for the rest of the receptor.

An extensive binding cavity is constructed from several structural elements. The cavity is enclosed from above by H5-6 (Met 256- Arg266), from below by H7 and H8 and the intervening loop (Leu287- Ile299), and along the sides by H2 (185- 187), by the turn between S3 and S4 (Leu276-Ser277), by H3 (Phe215-Arg228), by H11 (His381-Met388) and by H12 (Phe401-Phe405). The volume of the cavity defined by these elements, calculated by GRASP (Columbia University, USA) (600 Å3), is essentially the volume of the hormone (530 Å). The change in volume can be exploited for ligand design as described herein. The remaining volume is occupied by water molecules surrounding the amino-propionic acid substituent. FIG. 6 depicts various contacts (or interactions) between TR's LBD and the ligand.

The planes of the inner and outer (prime ring) rings of the ligand are rotated from planarity about 60° with respect to each other, adopting the 3'-distal conformation (in which the 3' substituent of the outer ring projects down and away 25 from the inner ring). The amino-propionic acid and the outer phenolic ring assume the transoid conformation, each on opposite sides of the inner ring. The torsion angle χ₁ for the amino- propionic acid is 300°.

The amino-propionic acid substituent is packed loosely in a polar pocket formed by side chains from H2, H4 and S3. The carboxylate group forms direct 30 hydrogen bonds with the guanidium group of Arg228 and the amino N of Ser277. In addition, Arg262, Arg266 and Asn179 interact with the carboxylate through water-mediated hydrogen bonds. The three arginine residues create a significantly positive local electrostatic potential, which may stabilize the negative charge of the

carboxylate. No hydrogen bond is formed by the amino nitrogen. The interactions of the amino-propionic acid substituent are consistent with the fact that Triac, which lacks the amino nitrogen, has a binding affinity equal to that of T₃, indicating that the amino nitrogen and longer aliphatic chain of T₃ do not contribute greatly to binding 5 affinity.

The biphenyl ether, in contrast, is found buried within the hydrophobic core. The inner ring packs in a hydrophobic pocket formed by H3, H5-6, and S3. Pockets for the 3- and 5-methyl substituents are not completely filled, as expected since the van der waals radius of methyl substituent for Dimit is smaller than the iodine substituent provided by the thyroid hormone T₃. Such pockets are typically 25 to 100 cubic angstroms (although smaller pocket for substitutes are contemplated in the 40 to 80 cubic angstrom range) and could be filled more tightly with better fitting chemical substitutions, as described herein.

The outer ring packed tightly in a pocket formed by H3, H5-6, H7, H8, H11 and H12, and the loop between H7 and H8. The ether oxygen is found in a hydrophobic environment defined by Phe218, Leu287, Leu276, and Leu292. The absence of a hydrogen bond to the ether oxygen is consistent with its role in establishing the correct stereochemistry of the phenyl rings, as suggested by potent binding of hormone analogs with structurally similar linkages possessing reduced or negligible hydrogen bonding capability. The 3'-isopropyl substituent contacts Gly290 and 291. The presence of glycine at this position in the pocket can explain the observed relationship between activity and the size of 3'-substituents. Activity is highest for 3'-isopropyl, and decreases with added bulk. The only hydrogen bond in the hydrophobic cavity is formed between the phenolic hydroxyl and His381 Ne2.

The conformation of His381 is stabilized by packing contacts provided by Phe405, and Met256.

The presence of a 5' substituent larger than hydrogen affects the binding affinity for hormone. The more abundant thyroid hormone, 3,5,3',5'-tetraiodo-L-thyronine (T₄), contains an iodine at this position, and binds the receptor with 2% of 30 the affinity of T₃. The structure suggests that discrimination against T₄ is accomplished through the combination of steric conflict by Met256 and possibly the constraints imposed by the geometry of the hydrogen bond from His381 to the phenolic hydroxyl. The 5' position is a preferred location for introducing a chemical

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modification of C-H at the 5' of T3 or and TR agonist, as described herein, that produces an extension from the prime ring and results in the creation of an antagonist or partial agonist.

Deletion and antibody competition studies suggest the involvement of residues

Pro162 to Val202 in ligand binding. The region does not directly contact hormone in
the bound structure, although H2 packs against residues forming the polar pocket that
interacts with the amino-propionic acid group. One role for H2, then, is to stabilize
these residues in the bound state, H2, with β-strands S3 and S4, might also represent a
prevalent entry point for ligand, since the amino-propionic acid of the ligand is
oriented toward this region. Studies of receptor binding to T3 affinity matrices
demonstrate that only a linkage to the amino-propionic acid is tolerated, suggesting
that steric hindrance present in other linkages prevent binding. Furthermore, the
crystallographic temperature factors suggest the coil and β-strand region is most
flexible part of the domain FIG. 7. Participation of this region, part of the hinge
domain between the DBD and LBD, in binding hormone may provide structural
means for ligand binding to influence DNA binding, since parts of the Hinge domain
contact DNA.

TR LBD Transcriptional Activation Helix As An Example Of A Nuclear Receptor 20 Activation Domain

In addition to the startling finding that the ligand binding cavity is solvent inaccessible when loaded with a ligand, the activation helix of TR LBD presents a surface to the ligand cavity for interaction between at least one amino acid and the bound ligand. The C-terminal 17 amino acids of the TR, referred to as the activation 25 helix or AF-2 (an example of an LBD activation domain), are implicated in mediating hormone-dependent transcriptional activation. Although, mutations of key residues within the domain decrease ligand-dependent activation it was unclear until the present invention whether such mutations directly affected ligand coordination. Although some mutations of this domain have been noted to reduce or abolish ligand 30 binding, other mutations in more distant sites of the LBD have a similar effect.

Activation domains among nuclear receptors display an analogous three dimensional relationship to the binding cavity, which is a region of the LBD that binds the molecular recognition domain of a ligand, i.e. the activation domain

presents a portion of itself to the binding cavity (but necessarily the molecular recognition domain of the ligand). Many nuclear receptors are expected to have such domains, including the retinoid receptors, RAR and RXR, the glucocorticoid receptor GR, and the estrogen receptor ER. Based upon the TR's sequence, the domain is proposed to adopt an amphipathic helical structure. β-sheet or mixed secondary structures, could be present as activation domains in less related nuclear receptors.

Within the activation domain, the highly conserved motif ΦΦΧΕΦΦ, where Φ represents a hydrophobic residue, is proposed to mediate interactions between the receptors and transcriptional coactivators. Several proteins have been identified which bind the TR in a hormone-dependent fashion. One of these, Trip1, is related to a putative yeast coactivator Sug1, and also interacts with both the C-terminal activation domain and a subset of the basal transcriptional machinery, suggesting a role in transactivation by the TR. Other proteins, such as RIP140, SRC1, (Onate, S.A. et. al., Science 270:1354-1357 (1995)) and TF-1 (see also Ledouarim, B., et. al., 15 EMBO J. 14:2020-2033 (1995)), and GRIP-1 (Heery, E., et al., Nature 387:733-736 (1997)) also interact with other nuclear receptors in a ligand dependent manner through the C-terminal domain. Binding of these proteins can be modulated using the TR ligands described herein especially those TR ligands with extensions that sterically hinder the interaction between the highly conserved motif and other 20 proteins.

The C-terminal activation domain of the TR forms an amphipathic helix, H12, which nestles loosely against the receptor to form part of the hormone binding cavity. The helix packs with the hydrophobic residues facing inward towards the hormone binding cavity, and the charged residues, including the highly-conserved glutamate, extending into the solvent, as shown in FIG. 8. The activation helix of TR LBD presents Phe 401 to the ligand binding cavity and permits direct coordination with the hormone i.e. such amino acids interact with the ligand forming a van der waals contact with the plane of the outer phenyl ring. Phe 405 also interacts with His 381, perhaps stabilizing its hydrogen bonding conformation, i.e. a favorable hydrogen bond interaction. Participation of Phe 401 and Phe 405 in binding hormone explains how mutation of these residues decreases hormone binding affinity. Furthermore, the impact of these mutations on activation likely derives from a role in stabilizing the domain in the bound structure through increased hydrogen bond interaction of dipole

interactions. Glu 403 extends into the solvent, emphasizing its critical role in transactivation. In its observed conformation, presented on the surface as an ordered residue, against a background of predominantly hydrophobic surface, Glu 403 is available to interact with activator proteins described herein, as shown in FIG. 9. The other charged residues, Glu 405 and Asp 406 are disordered, as the helix frays at Phe 405.

Two other sequences in the TR, τ2 and τ3, activate transcription when expressed as fusion proteins with a DNA-binding domain. The sequences, discovered in the TRB, correspond to TR-α residues Pro158-Ile168 in H1 (τ2), and Gly290-Leu3 10 19 in H8 and H9 (τ3). Unlike the C-terminal activation domain, τ2 and τ3 do not appear to represent modular structural units in the rat TR-I LBD, nor present a surface for protein-protein interactions: the critical aspartate/glutamate residues of τ3 are located on two separate helices, and do not form a single surface; the charged residues of τ2 are engaged in ion pair interactions with residues of the LBD. Thus, τ2 and τ3 may not function as activation domains in the context of the entire receptor.

Computational Methods For Designing A Nuclear Receptor LBD LIGAND

The elucidation of the three dimensional structure of a nuclear receptor ligand binding domain provides an important and useful approach for designing ligands to nuclear receptors using the computational methods described herein. By inspecting the FIGURES it can be determined that the nuclear receptor ligand is bound in a water inaccessible binding cavity in the LBD and that chemical moieties can be added to selected positions on the ligand. Such chemical modifications, usually extensions, can fill up the binding cavity represented in the FIGURES for a tighter fit (or less water) or can be used to disrupt or make contacts with amino acids not in contact with the ligand before the chemical modification was introduced or represented in a figure of the three dimensional model of the LBD. Ligands that interact with nuclear superfamily members can act as agonists, antagonists and partial agonists based on what ligand-induced conformational changes take place.

Agonists induce changes in receptors that place them in an active conformation that allows them to influence transcription, either positively or negatively. There may be several different ligand-induced changes in the receptor's conformation.

Antagonists, bind to receptors, but fail to induce conformational changes that alter the receptor's transcriptional regulatory properties or physiologically relevant conformations. Binding of an antagonist can also block the binding and therefore the actions of an agonist.

Partial agonists bind to receptors and induce only part of the changes in the receptors that are induced by agonists. The differences can be qualitative or quantitative. Thus, a partial agonist may induce some of the conformation changes induced by agonists, but not others, or it may only induce certain changes to a limited extent.

10

Ligand-induced Conformational Changes

As described herein, the unliganded receptor is in a configuration that is either inactive, has some activity or has repressor activity. Binding of agonist ligands induces conformational changes in the receptor such that the receptor becomes more active, either to stimulate or repress the expression of genes. The receptors may also have non-genomic actions. Some of the known types of changes and/or the sequelae of these are listed herein.

Heat Shock Protein Binding

For many of the nuclear receptors ligand binding induces a dissociation of heat shock proteins such that the receptors can form dimers in most cases, after which the receptors bind to DNA and regulate transcription.

Nuclear receptors usually have heat shock protein binding domains that present a region for binding to the LBD and can be modulated by the binding of a 25 ligand to the LBD. Consequently, an extended chemical moiety (or more) from the ligand that stabilizes the binding or contact of the heat shock protein binding domain with the LBD can be designed using the computational methods described herein to produce a partial agonist or antagonist. Typically such extended chemical moieties will extend past and away from the molecular recognition domain on the ligand and 30 usually past the buried binding cavity of the ligand.

Dimerization and Heterodimerization

With the receptors that are associated with the hsp in the absence of the ligand, dissociation of the hsp results in dimerization of the receptors. Dimerization is due to

receptor domains in both the DBD and the LBD. Although the main stimulus for dimerization is dissociation of the hsp, the ligand-induced conformational changes in the receptors may have an additional facilitative influence. With the receptors that are not associated with hsp in the absence of the ligand, particularly with the TR, ligand 5 binding can affect the pattern of dimerization/heterodimerization. The influence depends on the DNA binding site context, and may also depend on the promoter context with respect to other proteins that may interact with the receptors. A common pattern is to discourage monomer formation, with a resulting preference for heterodimer formation over dimer formation on DNA.

Nuclear receptor LBDs usually have dimerization domains that present a region for binding to another nuclear receptor and can be modulated by the binding of a ligand to the LBD. Consequently, an extended chemical moiety (or more) from the ligand that disrupts the binding or contact of the dimerization domain can be designed using the computational methods described herein to produce a partial agonist or antagonist. Typically such extended chemical moieties will extend past and away from the molecular recognition domain on the ligand and usually past the buried binding cavity of the ligand.

DNA Binding

20 In nuclear receptors that bind to hsp, the ligand-induced dissociation of hsp with consequent dimer formation allows, and therefore, promotes DNA binding. With receptors that are not associated (as in the absence of ligand), ligand binding tends to stimulate DNA binding of heterodimers and dimers, and to discourage monomer binding to DNA. However, ligand binding to TR, for example, tends to 25 decrease dimer binding on certain DNA elements and has minimal to no effect on increasing heterodimer binding. With DNA containing only a single half site, the ligand tends to stimulate the receptor's binding to DNA. The effects are modest and depend on the nature of the DNA site and probably on the presence of other proteins that may interact with the receptors. Nuclear receptors usually have DBDs that 30 present a region for binding to DNA and this binding can be modulated by the binding of a ligand to the LBD. Consequently, an extended chemical moiety (or more) from the ligand that disrupts the binding or contact of the DBD can be designed using the computational methods described herein to produce a partial agonist or antagonist. Typically such extended chemical moieties will extend past and away from the

molecular recognition domain on the ligand and usually past the buried binding cavity of the ligand.

Repressor Binding

Receptors that are not associated with hsp in the absence of ligand frequently act as transcriptional repressors in the absence of the ligand. This appears to be due, in part, to transcriptional repressor proteins that bind to the LBD of the receptors. Agonist binding induces a dissociation of these proteins from the receptors. This relieves the inhibition of transcription and allows the transcriptional transactivation functions of the receptors to become manifest.

Transcriptional Transactivation Functions

Ligand binding induces transcriptional activation functions in two basic ways. The first is through dissociation of the hsp from receptors. This dissociation, with consequent dimerization of the receptors and their binding to DNA or other proteins in the nuclear chromatin allows transcriptional regulatory properties of the receptors to be manifest. This may be especially true of such functions on the amino terminus of the receptors.

The second way is to alter the receptor to interact with other proteins involved 20 in transcription. These could be proteins that interact directly or indirectly with elements of the proximal promoter or proteins of the proximal promoter. Alternatively, the interactions could be through other transcription factors that themselves interact directly or indirectly with proteins of the proximal promoter. Several different proteins have been described that bind to the receptors in a ligand-25 dependent manner. In addition, it is possible that in some cases, the ligand-induced conformational changes do not affect the binding of other proteins to the receptor, but do affect their abilities to regulate transcription.

Nuclear receptors or nuclear receptor LBDs usually have activation domains modulated in part by a co-activator/co-repressor system that coordinately functions to 30 present a region for binding to DNA, and can be modulated by the binding of a ligand to the LBD. Consequently, an extended chemical moiety (or more) from the ligand that disrupts the binding or contact of the activation domain with co-activator and/or co-repressor can be designed using the computational methods described herein to produce a partial agonist or antagonist. For instance, an agonist can be designed

and/or selected which (1) blocks binding and/or dissociates co-repressor, and/or (2) promotes binding and/or association of a co-activator. An antagonist can be designed which (1) promotes binding and/or association of co-repressor, and/or (2) promotes binding and/or association of co-activator. Ratios of agonists and antagonists may be 5 used to modulate transcription of the gene of interest. Selection can be accomplised in binding assays that screen for ligands having the desired agonist or antagonist properties, including such ligands which induce conformational changes as decribed below. Suitable assays for such screening are described herein and in Shibata, H., et al. (Recent Prog. Horm. Res. 52:141-164 (1997)); Tagami, T., et al. (Mol. Cell Biol. 10 17(5):2642-2648 (1997)), Zhu, XG., et al. (J. Biol. Chem. 272(14):9048-9054 (1997)); Lin, B.C., et al. (Mol. Cell Biol. 17(10):6131-6138 (1997)); Kakizawa, T., et al. (J. Biol. Chem. 272(38):23799-23804 (1997)); and Chang, K. H., et al. (Proc. Natl. Acad. Sci. USA 94(17):9040-9045 (1997)). Typically such extended chemical moieties will extend past and away from the molecular recognition domain on the 15 ligand and usually past the buried binding cavity of the ligand and in the direction of the activation domain, which is often a helix as seen in the three dimensional model shown in the FIGURES in two dimensions on paper or more conveniently on a computer screen.

20 Ligand-Induced Conformational Change

Plasma proteins bind hormones without undergoing a conformational change through a static binding pocket formed between monomers or domains. For example, the tetrameric thyroid-binding plasma protein transthyretin forms a solvent-accessible hormone-binding channel at the oligomer interface. The structure of the protein is unchanged upon binding hormone with respect to the appearance of a buried binding cavity with a ligand bound.

However, the structural role for a ligand bound to a nuclear receptor LBD, like rat TR-α LBD, predicts that the receptor would differ in the bound and unbound states. In the absence of hormone, the receptor would possess a cavity at its core, 30 uncharacteristic of a globular protein. A ligand (e.g. hormone) completes the hydrophobic core of the active receptor after it binds to the nuclear receptor. Ligand binding by the receptor is a dynamic process, which regulates receptor function by inducing an altered conformation.

An exact description of the hormone-induced conformational changes requires comparison of the structures of the liganded and the unliganded TR. The structure of the unliganded human RXRα may substitute as a model for the unliganded TR. The rat TR-α LBD and human RXRα LBDs adopt a similar fold, and it is likely that the structural similarity extends to the conformational changes after ligand binding.

There are three major differences between the two structures, which indeed appear to be the result of ligand binding. First, the bound rat TR-α LBD structure is more compact, with the hormone tightly packed within the hydrophobic core of the receptor. By contrast, the unliganded human RXRα LBD contains several internal hydrophobic cavities. The presence of such cavities is unusual in folded proteins, and is likely a reflection of the unliganded state of the receptor. Two of these cavities were proposed as possible binding sites for 9-cis retinoic acid, though these multiple sites only partly overlap with the single buried binding cavity observed in the liganded rat TR-α LBD.

15 The second difference involves H11 in the rat TR-α LBD, which contributes part of the hormone binding cavity. H11, continuous in the rat TR-α LBD, is broken at Cys 432 in the RXR, forming a loop between H10 and H11 in the hRXRα. This residue corresponds to His381 in the TR, which provides a hydrogen bond to the outer ring hydroxyl of the ligand. Furthermore, the hormone binding cavity occupied by ligand in the rat TR-α LBD is interrupted in the hRXRα by the same loop, forming an isolated hydrophobic pocket in the RXR with H6 and H7. In the bound rat TR-α LBD, the corresponding helices H7 and H8 are contiguous with the binding pocket, and enclose the hormone binding cavity from below.

The third difference between the two receptors is the position of the C-25 terminal activation domain. While the C-terminal activation domain forms α-helices in both receptors, the domain in the rat TR-α LBD follows a proline-rich turn, and lies against the receptor to contribute part of the binding cavity. In contrast, the activation domain in the unliganded hRXRα, is part of a longer helix which projects into the solvent.

These differences lead to a model for an alternate conformation of the TR LBD assumed in the absence of ligand. In the unliganded TR, the subdomain of the receptor surrounding the hormone binding cavity is loosely packed, with the binding cavity occluded by a partly unstructured H11 providing a partial core for the receptor.

Upon binding hormone, residues which form a coil in the unbound receptor engage the ligand, and continues H11. The ordering of H11 could unblock the hydrophobic cavity, allowing H7 and H8 to interact with hormone. The extended hydrophobic cavity then collapses around the hormone, generating the compact bound 5 structure.

It is possible to predict ligand-induced conformational changes in the C-terminal activation domain that rely, in part, on an extended structure in the unliganded TR that repacks upon ligand binding. The ligand- induced conformation change can be subtle since the amino acid sequence of the rat TR-α in the turn (393-10 PTELFPP-399) significantly reduces the propensity of the peptide chain of the rat TR-α to form an α-helix and therefore repacking can be accomplished with a minor change in volume.

After the ligand-induced conformational change occurs, it is likely that the conformation of the C-terminal activation domain in the bound structure changes 15 packing compared to the unbound form of the receptor. Binding of the ligand improves the stability of the activation domain. The activation domain packs loosely even in the bound structure, as measured by the distribution of packing interactions for the entire LBD. The packing density for the activation domain, defined as the number of atoms within 4.5Å, is 1.5 standard deviations below the mean. For 20 comparison, another surface helix, H1, is 0.5 standard deviations below the mean and the most poorly packed part of the structure, the irregular coil from residues Ile196-Asp206, is 2.0 standard deviations below the mean. Moreover, the majority of packing contacts for the C-terminal domain in the bound receptor are provided either by residues which interact with ligand, such as His381, or by the ligand itself. The 25 conformation of these residues can be expected to be different in the bound and unbound receptors, and by extension the conformation of C-terminal activation domain which relies upon these interactions. Without the stabilization provided by a bound ligand, it is likely that the C-terminal activation domain is disordered prior to hormone binding.

The interrelation of ligand-induced conformational changes is evident as described herein. For example, His381 from H11 and Phe405 from H12 interact in the bound structure to provide a specific hydrogen bond to the phenolic hydroxyl. The

ligand-induced changes which affect H11 and H12 are reinforcing, and lead to the formation of the compact, bound state.

Comparison of the TR- α and TR- β LBD structures shows similar packing of the helices when complexed with the ligand Triac.

5

COMPUTATIONAL METHODS USING THREE DIMENSIONAL MODELS AND EXTENSIONS OF LIGANDS

The three-dimensional structure of the liganded TR receptor is unprecedented, and will greatly aid in the development of new nuclear receptor synthetic ligands, 10 such as thyroid receptor antagonists and improved agonists, especially those that bind selectively to one of the two TR isoforms (α or β). In addition, this receptor superfamily is overall well suited to modern methods including three-dimensional structure elucidation and combinatorial chemistry such as those disclosed in EP 335 628, U.S. patent 5,463,564, which are incorporated herein by reference. Structure 15 determination using X-ray crystallography is possible because of the solubility properties of the receptors. Computer programs that use crystallography data when practicing the present invention will enable the rational design of ligand to these receptors. Programs such as RASMOL can be used with the atomic coordinates from crystals generated by practicing the invention or used to practice the invention by 20 generating three dimensional models and/or determining the structures involved in ligand binding. Computer programs such as INSIGHT and GRASP allow for further manipulation and the ability to introduce new structures. In addition, high throughput binding and bioactivity assays can be devised using purified recombinant protein and modern reporter gene transcription assays described herein and known in the art in 25 order to refine the activity of a CDL.

Generally the computational method of designing a nuclear receptor synthetic ligand comprises two steps:

- determining which amino acid or amino acids of a nuclear receptor LBD interacts with a first chemical moiety (at least one) of the ligand using a three
 dimensional model of a crystallized protein comprising a nuclear receptor LBD with a bound ligand, and
 - 2) selecting a chemical modification (at least one) of the first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an

interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the first chemical moiety.

As shown herein, interacting amino acids form contacts with the ligand and 5 the center of the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer as discussed herein and in McRee 1993, however distances can be determined manually once the three dimensional model is made. Examples of interacting amino acids are described in Appendix 2. See also Wagner et al., Nature 10 378(6558):670-697 (1995) for stereochemical figures of three dimensional models. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. The invention can be practiced by repeating steps 1 and 2 to refine the fit of the ligand to the LBD and to determine a better ligand, such as an agonist. As shown in the FIGURES the three dimensional model of TR can be 15 represented in two dimensions to determine which amino acids contact the ligand and to select a position on the ligand for chemical modification and changing the interaction with a particular amino acid compared to that before chemical modification. Structural comparison of LBD isoforms complexed with the same or similar ligand permit identification of fiducial and adjustable amino acids that can be 20 exploited in designing isoform-specific ligands through chemical modification. "Fiducial" refers to amino acids that form rigid features of the ligand binding cavity. "Adjustable" refers to amino acids that form less rigid features of the ligand binding cavity. The chemical modification may be made using a computer, manually using a two dimensional representation of the three dimensional model or by chemically 25 synthesizing the ligand. The three dimensional model may be made using Appendix 2 and the FIGURES. As an additional step, the three dimensional model may be made using atomic coordinates of nuclear receptor LBDs from crystallized protein as known in the art, see McRee 1993 referenced herein.

The ligand can also interact with distant amino acids after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make as new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand. Often distant

amino acids will not line the surface of the binding cavity for the ligand, as they are too far away from the ligand to be part of a pocket or surface of the binding cavity.

The interaction between an atom of a LBD amino acid and an atom of an LBD ligand can be made by any force or attraction described in nature. Usually the 5 interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der waals interaction or dipole interaction. In the case of the hydrophobic interaction it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic group 10 from a hydrophobic surface. Reduction or enhancment of the interaction of the LBD and a ligand can be measured by standard binding procedures, calculating or testing binding energies, computationally or using thermodynamic or kinetic methods as known in the art.

Chemical modifications will often enhance or reduce interactions of an atom of a LBD amino acid and an atom of an LBD ligand. Steric hinderance will be a common means of changing the interaction of the LBD binding cavity with the activation domain. Chemical modifications are preferably introduced at C-H, C- and C-OH position in ligands, where the carbon is part of the ligand structure which remains the same after modification is complete. In the case of C-H, C could have 1, 2 or 3 hydrogens, but usually only one hydrogen will be replaced. The H or OH are removed after modification is complete and replaced with the desired chemical moiety.

Because the thyroid receptor is a member of the larger superfamily of hormone-binding nuclear receptors, the rules for agonist and antagonist development will be recognized by one skilled in the art as useful in designing ligands to the entire superfamily. Examining the structures of known agonists and antagonists of the estrogen and androgen receptors supports the generality of antagonist mechanism of action as shown in **FIG. 10**.

The overall folding of the receptor based on a comparison of the reported structure of the unliganded RXR and with amino acid sequences of other superfamily members reveals that the overall folding of receptors of the superfamily is similar. Thus, it is predicted from the structure that there is a general pattern of folding of the nuclear receptor around the agonist or antagonist ligand.

The three dimensional structure of a nuclear receptor with a ligand bound leads to the nonobvious observation that a nuclear receptor folds around agonist ligands, as the binding cavity fits the agonist, especially the agonist's molecular recognition domain, and antagonists commonly have chemical structures that extend 5 beyond the ligand, especially the agonist, and would prohibit folding of the receptor around the ligand to form a buried binding cavity or other groups that have the same effect. The location of the extension could affect the folding in various ways as indicated by the structure. Such extensions on antagonists are shown in FIG. 10 for various receptors and compared to the corresponding agonist.

10 For example, an extension towards the carboxy-terminal activation helix affects the packing/folding of this helix into the body of the receptor. This in turn can affect the ability of this portion of the nuclear receptor to interact with other proteins or other portions of the receptor, including transcriptional transactivation functions on the opposite end of the linear receptor, or the receptor's amino terminus that may 15 interact directly or indirectly with the carboxy-terminal transactivation domain (including helix 12). Extensions in this direction can also affect the packing of helix 11 of TR (or its analogous helix in nuclear receptors) into the body of the receptor and selectively affect dimerization and heterodimerization of receptors. An extension pointing towards helix 1 can affect the relationship of the DNA binding domain and 20 hinge regions of the receptors with the ligand binding domain and selectively or in addition affect the receptors' binding to DNA and/or interactions of receptors with proteins that interact with this region of the receptor. Other extensions towards helix 11 can be made to affect the packing of this helix and helices 1 and 10 and thereby homo- and hetero-dimerization. Such chemical modifications can be assessed using 25 the computational methods described herein. It is also possible that, in some cases, extensions may protrude through the receptor that is otherwise completely or incompletely folded around the ligand. Such protruding extensions could present a steric blockade to interactions with co-activators or other proteins.

The three dimensional structure with the ligand buried in the binding cavity immediately offers a simple description of a nuclear receptor that has a binding cavity that contains hinges and a lid, composed of one or more structural elements, that move to accommodate and surround the ligand. The ligand to TR can be modified on specific sites with specific classes of chemical groups that will serve to leave the lid and hinge region in open, partially open or closed states to achieve partial agonist or

antagonist functions. In these states, the biological response of the TR is different and so the structure can be used to design particular compounds with desired effects.

Knowledge of the three-dimensional structure of the TR-T₃ complex leads to a general model for agonist and antagonist design. An important novel feature of the structural data is the fact that the T₃ ligand is completely buried within the central hydrophobic core of the protein. Other ligand-receptor complexes belonging to the nuclear receptor superfamily will have a similarly buried ligand binding site and therefore this model will be useful for agonist/antagonist design for the entire superfamily.

When design of an antagonist is desired, one needs either to preserve the important binding contacts of natural hormone agonist while incorporating an "extension group" that interferes with the normal operation of the ligand-receptor complex or to generate the requisite binding affinity through the interactions of the extensions with receptor domains.

15 The model applied to antagonist design and described herein is called the "Extension Model." Antagonist compounds for nuclear receptors should contain the same or similar groups that facilitate high-affinity binding to the receptor, and in addition, such compounds should contain a side chain which may be large and/or polar. This side chain could be an actual extension, giving it bulk, or it could be a 20 side group with a charge function that differs from the agonist ligand. For example, substitution of a CH₃ for CH₂OH at the 21-position, and alteration at the 11-position from an OH group to a keto group of cortisol generates glucocorticoid antagonist activity (Robsseau, G.G., et. al., J. Mol. Biol. 67:99-115 (1972)). However, in most cases effective antagonists have more bulky extensions. Thus, the antiglucocorticoid 25 (and antiprogestin) RU486 contains a bulky side group at the 11-position (Horwitz, K.B. Endocrine Rev. 13:146-163 (1992)). The antagonist compound will then bind within the buried ligand binding site of the receptor with reasonably high affinity (100 nM), but the extension function will prevent the receptor-ligand complex from adopting the necessary conformation needed for transcription factor function. The 30 antagonism (which could be in an agonist or antagonist) may manifest itself at the molecular level in a number of ways, including by preventing receptor homo/heterodimer formation at the HRE, by preventing coactivator binding to receptor monomers, homodimers or homo/heterodimers, or by a combination of these effects which otherwise prevent transcription of hormone responsive genes mediated

by ligand-induced effects on the HRE. There are several antagonist compounds for nuclear receptors in the prior art (see also Horwitz, K.B., Endocrine Rev. 13:146-163 (1992), Raunnaud J.P. et. al., J. Steroid Biochem. 25:811-833 (1986), Keiel S., et. al., Mol. Cell. Biol. 14:287-298 (1994) whose antagonist function can be explained by the extension hypothesis. These compounds are shown in FIG. 10 along with their agonist counterparts. Each of these antagonists contains a large extension group attached to an agonist or agonist analogue core structure. Importantly, these antagonist compounds were discovered by chance and not designed with a structure-function hypothesis such as the extension principle.

One method of design of a thyroid antagonist using the extension hypothesis is provided below as a teaching example. The three-dimensional structure of the TR-α Dimit complex combined with structure-activity data published in the prior art, especially those reference herein, can be used to establish the following ligand-receptor interactions which are most critical for high-affinity ligand binding.

15 A physical picture of these interactions is shown in FIG. 6. The figure describes the isolated essential contacts for ligand binding. Because the ligand is buried in the center of the receptor, the structural spacing between these isolated interactions is also important. Thus, our present knowledge of this system dictates that, for this example, a newly designed ligand for the receptor must contain a thyronine structural skeleton, or two substituted aryl groups joined by a one-atom spacer.

The general structure for an antagonist designed by the extension hypothesis is exemplified in the following general description of the substituents of a TR antagonist (referring to Formula 1): R₁ can have anionic groups such as a carboxylate, phosphonate, phosphate, sulfate or sulfite and is connected to the ring with a 0 to 3 atom linker, comprising one or more C, O, N, S atoms, and preferably a 2 carbon linker. Such R₁ can be optionally substituted with an amine (e.g. -NH₂). R₃ and R₅ are small hydrophobic groups such as -Br, -I, or -CH₃. R₃ and R₅ can be the same substituents or different. R₃' can be a hydrophobic group that may be larger than those of R₃ and R₅, such as -I, -CH₃, -isopropyl, -phenyl, -benzyl, 5 and 6 ring heterocycles. R₄' is a group that can participate in a hydrogen bond as either a donor or acceptor. Such groups include -OH, -NH₂, and -SH. R₅' is an important extension group that makes this compound an antagonist. R₅' can be a long chain alkyl (e.g. 1 to 9 carbons, straight chain or branched), aryl (benzyl, phenyl and substituted benzyl

and phenyl rings (e.g. with halogen, alkyl (1 and 5 carbons) and optionally connected to the ring by a -CH₂-), heterocycle (e.g. 5 or 6 atoms, preferably 5 carbons and 1 nitrogen, or five carbons), which can optionally include polar (e.g. -OH, -NH₂, and -SH), cationic (e.g. -NH₃, N(CH)₃), or anionic (carboxylate, phosphonate, phosphate or sulfate) groups. R₅' can also be a polar (e.g. -OH, -NH₂, and -SH), cationic (e.g. -NH₃, -N(CH₃)₃), and anionic (carboxylate, phosphonate, phosphate or sulfate) groups. X is the spacer group that appropriately positions the two aromatic rings. This group is usually a one-atom spacer, such as O, S, SO, SO₂, NH, NZ where Z is an alkyl, CH₂, CHOH, CO, C(CH₃)OH, and C(CH₃)(CH₃). X also may be NR₇, CHR₇, CR₇, R₇, where R₇, is an alkyl, aryl or 5- or 6-membered heterocyclic aromatic. R₂, R₆, R₂' and R₆' can be -F, and -Cl and are preferably H.

A TR ligand can also be described as a substituted phenylated 3,5 diiodo tyrosine with substituted R₅' and R₃' groups. R₅' can be a long chain alkyl (e.g. 4 to 9 carbons, straight chain or branched), aryl (benzyl, phenyl and substituted benzyl and 15 phenyl rings (e.g with halogen, alkyl (1 and 5 carbons) and optionally connected to the ring by a -CH₂-), heterocycle (e.g. 5 or 6 atoms, preferably 5 carbons and 1 nitrogen, or five carbons), which can optionally include polar (e.g. -OH, -NH₂, and -SH), cationic (e.g. -NH₃, N(CH)₃), or anionic (carboxylate, phosphonate, phosphonate or sulfate) groups. R₅' can also be a polar (e.g. -OH, -NH₂, and -SH), cationic (e.g. - NH₃, N(CH)₃), and anionic (carboxylate, phosphonate, phosphate or sulfate) groups. R₃' can be -IsoPr, halogen, -CH₃, alkyl (1 to 6 carbons) or aryl (benzyl, phenyl and substituted benzyl and phenyl rings (e.g with halogen, alkyl (1 and 5 carbons) and optionally connected to the ring by a -CH₂-), heterocycle (e.g. 5 or 6 atoms, preferably 5 carbons and 1 nitrogen, or five carbons), which can optionally include polar (e.g. - 25 OH, -NH₂, and -SH), cationic (e.g. -NH₃, N(CH)₃), or anionic (carboxylate, phosphonate, phosphate or sulfate) groups.

A TR antagonist can also be a modified T₃ agonist (having a biphenyl structure) wherein R₅' is alkyl, aryl, 5- or 6-membered heterocyclic aromatic, heteroalkyl, heteroaryl, arylalkyl, heteroaryl alkyl, polyaromatic, polyheteroaromatic, 30 polar or charged groups, wherein said R₅' may be substituted with polar or charged groups. The R₅' groups are defined, as described herein.

Using these methods the ligands of this example preferably have the following properties:

1. The compounds should bind to the TR with high affinity (for example 100 nM).

- 2. The compounds should bind the receptor in the same basic orientation as the natural hormone.
- 5 3. The extension group R_5 ' should project toward the activation helix (C-terminal helix) of the receptor.
 - 4. The appropriate substituent at R_5 ' should perturb the activation helix from its optimal local structure needed for mediating transcription.

Antagonists may also be designed with multiple extensions in order to block 10 more than one aspect of the folding at any time.

TR ligands (e.g. super agonists) can be designed (and synthesized) to enhance the interaction of at least one amino acid with at least one chemical moiety on the ligand's molecular recognition domain. One method is to enhance the charge and polar interactions by replacing the carboxylate of T₃ (R₁ position) with phosphonate, 15 phosphate, sulfate or sulfite. This enhances the interaction with Arg 262, Arg 266 and Arg 228. The interaction of at least one amino acid with at least one chemical moiety on the ligand's molecular recognition domain can also be enhanced by increasing the size of R₁ group to fill the space occupied by water when Dimit is bound (referring to R₁). Preferably the group has a complementary charge and hydrophobicity to the binding cavity.

Another way of improving the interaction of at least one amino acid with at least one chemical moiety on the ligand's molecular recognition domain is to restrict the conformation of the dihedral angle between the two phenyl rings of the thyronine ligand in solution. In solution the planes of two phenyl rings are orthogonal where the dihedral angle is 90°. In the TR Dimit structure, the dihedral angle is close to 60°. A TR ligand design that fixes the angle between the two phenyl rings will lead to tighter binding. Such a ligand may be made by connecting the R₆' and the R₅ positions of a thyronine or a substituted thyronine-like biphenyl. The size of the cyclic connection can fix the angle between the two phenyl rings. Referring specifically to Formula 1, 30 the following cyclic modifications are preferred: 1) R₅ is connected to R₆', 2) R₃ is connected to R₂' or 3) R₅ is connected to R₆' and R₃ is connected to R₂'. The connections can be made by an alkyl or heteroalkyl chain having between 1 to 6 atoms and preferably from 2 to 4 carbon atoms or other atoms. Any position of the heteroalkyl chain can be N, O, P or S. The S and P heteroatoms along said heteroalkyl

chain are in any of their possible oxidative states. The N heteroatom or any carbon along the alkyl or heteroalkyl chain may have one or more Z substituents, wherein Z is alkyl, heteroalkyl, aryl, heteroaryl, 5- or 6-membered heterocyclic aromatic. These compounds can be claimed with the proviso that Formula 1 does not include any prior art compound as of the priority filing date of this application.

The interaction of at least one amino acid with at least one chemical moiety on the ligand's molecular recognition domain can also be enhanced by selecting a chemical modification that fills the unfilled space between a TR ligand and the LBD in the area of the bridging oxygen (such as in T3, Triac or Dimit). Thus, a slighter larger moiety that replaces the ether oxygen can enhance binding. Such a linker may be a mono- or geminal- disubstituted carbon group. A group approximately the same size as oxygen but with greater hydrophobicity is preferred as well as small, hydrophobic groups for the disubstituted carbon.

Compounds of Formula I or derivatives thereof that modulate TR activity also 15 may be designed and selected to interact with a conformationally constrained structural feature of a TR LBD that is conserved among TR LBD isoforms to increase TR-specific selectivity. Conserved structural features of a TR LBD include residues found in equivalent positions of TR LBD isoforms which interact with a conserved structural feature of a compound comprising the biphenyl scaffold (φ-X-φ) or a single 20 phenyl scaffold (φ-X or X-φ) of Formula I. Conformationally constrained structural features of a TR LBD include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-ligand recognition and binding. 25 For example, comparison of atomic models of TR LBD isoforms bound to thyronine and thyronine-like ligands reveal that certain residues which contact the ligands are restricted to particular topological shapes and angles of rotation about bonds. These include Met259, Leu276, Leu292, His381, Gly290, Ile221, and Phe401 of TR-a. The corresponding positions in TR-β include Met313, Leu330, Leu346, His435, Gly344,

Selectivity imparted by conformationally constrained features of both the receptor and compound are of particular interest. For example, compounds of Formula I comprising constrained cyclic carbons and substituent groups that interact

30 Ile275 and Phe455, respectively.

with a constrained feature of a TR LBD can be exploited to further increase binding specificity while reducing the potential for cross-over interaction with other receptors. These include hydrophobic and/or hydrophilic contacts between constrained residues of a TR LBD and atomic groups of the following constituents of the compound in 5 reference to Formula I: (i) the biphenyl rings; (ii) the R₃-substituent; (iii) the R₃'-substituent; and (iv) the R₄'-substituent.

For example, contacts to the phenyl moiety comprising the R₁, R₂, R₃, R₅ and R₆ substituents, i.e., the ring proximal to the polar pocket (the "inner ring"), include a cycle carbon atom that interacts with an atom of a hydrophobic residue of a TR LBD, such as a carbon and oxygen atom of Met259 and a carbon atom of Leu276 of TR-α, or Met313 and Leu330 of TR-β, where the cycle carbon is about 3.0 to 4.0A from the atom of the hydrophobic group. For example, comparison of TR-α complexed with T3 and TR-β complexed with GC-1 reveals the following conserved inner ring contacts:

Ligand	TR LB	D	
T3/Atom	TR-α Residue	Atom	Distance
C11	Met259	С	3.95
C11	Met259	O	3.59
C11	Met259	CB	3.77
C7	Leu276	CD2	3.80
C9	Leu276	CD2	3.70
GC1/Atom	TR-β Residue	Atom	Distance
C11	Met313	С	3.85
C11	Met313	O	3.41
C11	Met313	CB	3.79
C7	Leu330	CD2	3.56
C9	Leu330	CD2	3.63
	T3/Atom C11 C11 C11 C7 C9 GC1/Atom C11 C11 C11 C7	T3/Atom TR-α Residue C11 Met259 C11 Met259 C11 Met259 C7 Leu276 C9 Leu276 GC1/Atom TR-β Residue C11 Met313 C11 Met313 C11 Met313 C7 Leu330	T3/Atom TR-α Residue Atom C11 Met259 C C11 Met259 O C11 Met259 CB C7 Leu276 CD2 C9 Leu276 CD2 GC1/Atom TR-β Residue Atom C11 Met313 C C11 Met313 O C11 Met313 CB C7 Leu330 CD2

Contacts to the phenyl moiety comprising the R₂', R₃', R₄', R₅' and R₆' substituents, i.e., the ring distal to the polar pocket (the "outer ring"), include a cyclic carbon atom that interacts with an atom of a hydrophobic residue of a TR LBD, such 35 as a carbon atom of Leu292 of TR-α, or Leu346 of TR-β, where the cyclic carbon atom is about 3.0 to 4.0A from the atom of the hydrophobic residue. For example, comparison of TR-α complexed with T3 and TR-β complexed with GC-1 reveals the following conserved outer ring contacts:

	<u>Ligand</u>	TR LB	D	-
	T3/Atom	TR-α Residue	Atom	Distance
	C6	Leu292	CD2	3.58
	C8	Leu292	CD2	3.50
5	GC1/Atom	TR-β Residue	Atom	Distance
	C6	Leu346	CD2	3.77
	C8	Leu346	CD2	3.80

Contacts to the R₃-substituent include an atom that interacts with a carbon atom of a hydrophobic residue of a TR LBD, such as Ile221 of TR-α, or Ile275 of TR-β, where the R₃-substituent atom is about 3.0 to 4.0A from the carbon atom of the hydrophobic residue. For example, comparison of TR-α complexed with T3 and TR-β complexed with GC-1 reveals the following conserved R₃-substituent contacts:

15

	<u>Ligand</u>	TR LBD	
	T3/Atom I1	TR-α Residue At Ile221 CC	
20	GC1/Atom C19	TR-β Residue Ato	

Contacts to the R₃'-substituent include an atom that interacts with an atom of a hydrophobic or hydrophilic residue of a TR LBD, such as an oxygen atom of Gly290 25 of TR-α, or Gly344 of TR-β, where the R₃'-substituent atom is about 3.0 to 4.0A from the atom of the hydrophobic or hydrophilic residue. For example, comparison of TR-α complexed with T3 and TR-β complexed with GC-1 reveals the following conserved R₄'-substituent, phenolic hydroxyl contacts:

30	<u>Ligand</u>	TR LBD)	
	T3/Atom I2	TR-α Residue . Gly290	Atom O	Distance 3.50
	GC1/Atom C18	TR-β Residue A	Atom O	Distance 3.60

35

Contacts to the R_4 '-substituent comprising a phenolic hydroxyl include carbon and oxygen atoms that interact with a hydrophobic or hydrophilic residue of a TR LBD, such as a carbon and nitrogen atom of His381 of TR- α , or His435 of TR- β ,

where the R_4 '-substituent atom is about 2.0 to 4.0A from an atom of the hydrophobic or hydrophilic residue. For example, comparison of TR- α complexed with T3 and TR- β complexed with GC-1 reveals the following conserved R_4 '-substituent, phenolic hydroxyl contacts:

5			
	<u>Ligand</u>	TR LBD	_
	T3/Atom	TR-α Residue Atom	Distance
	C10	His381 CD2 3.97	
	O1	His381 CD2 3.39	
10	O1	His381 CE1 3.82	
	C8	His381 NE2 3.47	
	C10	His381 NE2 3.55	
	O1	His381 NE2 2.70	
	GC1/Atom	TR-β Residue Atom	Distance
15	C10	His435 CD2 3.89	
	O1	His435 CD2 3.64	
	01	His435 CE1 3.79	
	C8	His435 NE2 3.44	
	C10	His435 NE2 3.33	
20	O1	His435 NE2 2.77	

Contacts to the R₄'-substituent also may include an atom that interacts with a carbon atom of a hydrophobic residue of a TR LBD, such as Phe401 of TR-α, or 25 Phe455 of TR-β, for defining agonist activity, i.e., proper presentation of helix-12 (H12) of the TR LBD following ligand binding. The R₄'-substituent atom is about 3.0 to 4.0Å from the carbon atom of the hydrophobic group. For example, comparison of TR-α complexed with T3 and TR-β complexed with GC-1 reveals the following conserved R₄'-substituent contacts:

30				
	Ligand_	TR LB	D	
	T3/Atom	TR-α Residue	Atom	Distance
	O1 .	Phe401	CE1	3.52
	O1	Phe401	CZ	3.32
35	GC1/Atom	TR-β Residue	Atom	Distance
	O1	Phe455	CE1	3.40
	O1	Phe455	CZ	3.22

40 Comparison of atomic models of TR LBD isoforms complexed with the same and/or different ligands therefore facilitates the identification of new compounds that

fit spacially and preferentially into a TR LBD. Modeling, comparison of TR-ligand overlays, and comparison of TR LBD isoforms also permit identification of conformationally conserved structural features of TR LBD/ligand contacts. Exploiting conformational constraints of the LBD-ligand interaction identified by such methods therefore improves the design and identification of new compounds having increased selectivity for binding a particular type of nuclear receptor, such as TR.

TR-α AND TR-β SELECTIVITY FOR THE THYROID HORMONE RECEPTOR

Using the method described herein ligands can be designed that selectively bind to the alpha more than the beta TR or vice versa. The X-ray crystallographic structure of the rat TR-α LBD provides insight into design of such ligands.

The three dimensional structure reveals that the major difference between the TR-α and TR-β in the ligand binding cavity resides in amino acid Ser 277 (with the side group -CH₂OH) in the rat TR-α and whose corresponding residue is 331, asparagine (with the side group -CH₂CONH₂), in the human TR-β. The side chain in human TR-β is larger, charged and has a different hydrogen bonding potential, which would allow the synthesis of compounds that discriminate between this difference. The Ser277 (Asn331 in TR-β) forms part of the polar pocket of the TR LBD, indicating that for TR-α versus TR-β discrimination, ligands can be designed to contain chemical modification of the R1-substitutent with reference to Formula I that exploit this difference.

For example, in the complex of TR-α with Triac, Ser277 does not participate in ligand binding. The absence of a role for Ser277 (Asn331 in beta) is consistent 25 with the equal affinity of Triac for the alpha and beta isoforms, and indirectly supports the contention that alpha/beta selectivity resides in the amino acid substitution Ser277 to Asn331 and its interaction with Arg228. The effect of the amino acid substitution is further evident when the interactions of Asn331 and Arg282 in the structures of the TR-β LBD complexed with GC-1 or Triac are compared with those of Ser277 and Arg228 in the TR-α LBD. In the complex with GC-1, Asn331 forms a hydrogen bond to Arg282, which in turn forms a hydrogen bond with the carboxylate of GC-1, a pattern that resembles the interactions of Ser277 and Arg228 in the complexes of the TR-α LBD complexed with T₃ or Triac.

However, in the complex of TR-β with Triac, Arg282 rotates away from Asn331 and the ligand, instead forming hydrogen bonds to residues Thr287 and Asp291 of H3. Therefore, differences exist between the two isoforms in the conformation of the polar pocket, depending on the nature of the ligand R₁-substitutent, indicating that certain substituents may interact preferentially with the conformation of a given isoform.

Comparing overlays of various ligands bound to the TR-α versus TR-β LBDs shows the positioning of the ligand to be very similar. Surprisingly, comparison of the volume and area for the $TR-\alpha$ and $TR-\beta$ LBDs bound by the same or different ligands unexpectedly shows that the cubic space or volume available for 10 accommodating ligand binding by the TR- β LBD (645 ± 28.28 Å³) is larger and more flexable than that of the TR- α LBD (596.25 ± 7.97 Å³) (Table 1). The volume of the ligand binding cavity for TR-α varies over a narrow range of about 8+, with a maximum difference of about 16+. In contrast, the volume of the ligand binding cavity for TR-β differs by nearly 40+ between the complexes with GC-1 and Triac. 15 There also is a difference in the volume of the ligand binding cavity when comparing the same ligand bound to TR- α and TR- β . For example, TR- α and TR- β complexed with Triac differ in LBD volume by about 36 Å³. Comparison of TR-α and TR-β bound to Dimit and GC-1, respectively, which ligands have similar volume/area and superpositioned architecture, show that the difference in LBD volume is about 75 Å³. 20 These differences are attributed primarily to variable movement and interaction of side chain groups with ligand substitutents of the phenyl moiety (ϕ) of the biphenyl scaffold $(\phi - X - \phi)$ located proximal to the polar pocket, e.g., R_1 -substituents in reference to Formula I. In contrast, the volume available in the hydrophobic pocket for both the TR- α and TR- β LBDs is substantially the same. For example, binding of 25 Triac to the TR-β LBD displaces the side chain of Arg 282 providing approximately 60 Å³ in the polar pocket cavity, exposing the polar pocket to bulk solvent exchange. For GC-1 bound to the TR-β LBD, approximately 14 Å³ is due to side chain motion of Met310, and approximately 44 Å³ is due to side chain motion of Arg320, the combination of which increases the size of the polar pocket in the TR-β LBD. This 30 extra pliability also may explain the absence of ordered water in the polar pocket of TR-β LBD bound to Triac or GC-1, which is in contrast to the ordered water found in the polar pocket of TR- α LBD bound to Dimit, IpBr2 or T3.

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Table 1*

rTR-α						
	Dimit	Triac	IpBr2	T3		
TR LBD (volÅ ³ /areaÅ ²)	590/456	589/440	601/474	605/472		
Ligand (volÅ ³ /areaÅ ²)	303/314	333/326	326/330	355/346		
Complementarity	0.65	0.68	0.66	0.71		

	h'i	ΓR-β	
	GC-1	Triac	·
TR LBD (volų/areaŲ)	665/575	625/474	
Ligand (volÅ ³ /areaÅ ²)	294/310	333/326	
Complementarity	0.61	0.67	

*TR LBD volume and area are reported in Angstroms measured by GRASP. Complementarity is determined as defined in Lawrence *et al.*, *J. Mol. Biol. 234*:946-950 (1993).

Residue Ser277 in TR-α and the corresponding residue Asn331 of TR-β also contribute to the volumetric differences observed in the polar pockets of these two TR isoforms. And substitution of the Asn331 of hTR-β with serine has the affect of modifying ligand binding affinity of TR-β so that it resembles that of TR-α (See Example 5). Taken together, differences in hydrogen bonding of atoms of the side chain group of Ser277 in TR-α and Asp331 in TR-β extending from the equivalent backbone position in these TR LBDs and the more restricted polar pocket of the TR-α LBD further supports the concept of designing TR LBD isoform-specific ligands 15 having substitutents that fit spacially and preferentially into the polar pocket of either the TR-α or TR-β LBDs. Exploitation of this difference provides an additional means for computational design of isoform-specific TR agonists and antagonists.

In terms of ligand design, these differences mean that for β -selective ligands, some or all of the following differences should be exploited:

- 20 1. The presence of a larger side chain asparagine.
 - 2. The ability of the carbonyl group on the side chain to provide a strong hydrogen bond acceptor.
 - 3. The ability of the amido group on the side chain to provide a two hydrogen bond donors.
- 25 4. Adjustment of polarity to reorganize the trapped water in the T3 pocket.
 - 5. Greater size and flexibility of the polar pocket.

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In terms of pharmaceutical design, these differences mean that for α -selective ligands, some or all of the following differences should be exploited:

- 1. The presence of a smaller side group.
- 2. The ability of the hydroxyl on the -CH₂OH side group carbonyl group on the side chain to provide a weak hydrogen donor.
 - 3. Adjustment of polarity to reorganize the trapped water in the T3 pocket.
 - 4. Smaller size and limited flexibility of the polar pocket.

In both cases these differences can be exploited in a number of ways. For example, they can also be used with a software set for construction of novel organic molecules such as LUDI from Biosym-MSI. An example of designing TR-β selective ligands is increasing the polarity of a ligand substituent located in the polar pocket of a TR LBD through addition of one or more ligand groups having a formal negative charge and/or negative dipole charge that interacts with a formal positive charge and/or positive dipole charge of a group in the polar pocket of the LBD. This exploits preferential interactions, such as with the additional positive charge contributed by Asn 331 in TR-β. Another example of a TR-β selective ligand is one that comprises one or more groups which fit spacially into the TR-β LBD polar pocket. This exploits spacial differences between TR LBD isoforms, such as the larger and more flexible polar pocket of TR-β.

METHODS OF TREATMENT

The compounds of Formula 1 can be useful in medical treatments and exhibit biological activity which can be demonstrated in the following tests:

(i) the induction of mitochondrial α-glycerophosphate dehydrogenase (GPDH:EC 1.1.99.5). This assay is particularly useful since in certain species e.g. rats it is induced specifically by thyroid hormones and thyromimetics in a close-related manner in responsive tissues e.g. liver, kidney and the heart (Westerfield, W.W., Richert, D.A. and Ruegamer, W.R., Endocrinology (1965) 77:802). The assay allows direct measurement in rates of a thyroid hormone-like effect of compounds and in particular allows measurement of the direct thyroid hormone-like effect on the heart. Other measurements included parameters such as heart rate and cardiac

enzymes including Ca⁺⁺ ATPase, Na⁺⁺/K⁺ ATPase, myosin isoforms and specific liver enzymes;

- (ii) the elevation of basal metabolic rate as measured by the increase in whole body oxygen consumption (see e.g., Barker et al., Ann. N. Y. Acad. Sci., (1960)
 5 86:545-562);
 - (iii) the stimulation of the rate of beating of atria isolated from animals previously dosed with thyromimetrics (see e.g., Stephan *et al.*, *Biochem. Pharmacol.* (1992) 13:1969-1974; Yokoyama *et al.*, *J. Med. Chem.*, (1995) 38:695-707);
- (iv) the change in total plasma cholesterol levels as determined using a 10 cholesterol oxidase kit (for example, the Merck CHOD iodine colorimetric kit. see also, Stephan et al. (1992));
- (v) the measurement of LDL (low density lipoprotein) and HDL (high density lipoprotein) cholesterol in lipoprotein fractions separated by ultracentrifugation; and p (vi) the change in total plasma triglyceride levels as 15 determined using enzymatic color tests, for example the Merck System GPO-PAP method.

The compounds of Formula 1 can be found to exhibit selective thyromimetic activity in these tests,

- (a) by increasing the metabolic rate of test animals, and raising hepatic 20 GPDH levels at doses which do not significantly modify cardiac GPDH levels.
 - (b) by lowering plasma cholesterol and triglyceride levels, and the ratio of LDL to HDL cholesterol at doses which do not significantly modify cardiac GPDH levels.
- The compounds of Formula 1 may therefore be used in therapy, in the 25 treatment of conditions which can be alleviated by compounds which selectively mimic the effects of thyroid hormones in certain tissues whilst having little or no direct thyromimetic effect on the heart. For example, compounds of Formula 1 which raise hepatic GPDH levels and metabolic rate at doses which do not significantly modify cardiac GPDH levels are indicated in the treatment of obesity.
- Agonists of Formula 1 will lower total plasma cholesterol, the ratio of LDL-cholesterol to HDL-cholesterol and triglyceride levels at doses which do not significantly modify cardiac GPDH levels are indicated for use as general antihyperlipidaemic (antihyperlipoproteinaemic) agents i.e. in the treatment of patients having elevated plasma lipid (cholesterol and triglyceride) levels. In

addition, in view of this effect on plasma cholesterol and triglyceride, they are also indicated for use as specific anti-hypercholesterolemic and anti-hypertriglyceridaemic agents.

Patients having elevated plasma lipid levels are considered at risk of 5 developing coronary heart disease or other manifestations of atherosclerosis as a result of their high plasma cholesterol and/or triglyceride concentrations. Further, since LDL-cholesterol is believed to be the lipoprotein which induces atherosclerosis, and HDL-cholesterol believed to transport cholesterol from blood vessel walls to the liver and to prevent the build up of atherosclerotic plaque, anti-hyperlipidemic agents which lower the ratio of LDL-cholesterol to HDL cholesterol are indicated as anti-atherosclerotic agents, herein incorporated by reference U.S. patents 4,826,876 and 5,466,861.

The present invention also provides a method of producing selective thyromimetic activity in certain tissues except the heart which comprises administering to an animal in need thereof an effective amount to produce said activity of a compound of Formula 1 or a pharmaceutically acceptable salt thereof.

The present invention also relates to a method of lowering plasma lipid levels and a method of lowering the ratio of LDL-cholesterol to HDL-cholesterol levels by suitably administering a compound of this invention or a pharmaceutically acceptable 20 sale thereof.

In addition, compounds of Formula 1 may be indicated in thyroid hormone replacement therapy in patients with compromised cardiac function.

In therapeutic use the compounds of the present invention are usually administered in a standard pharmaceutical composition.

The present invention therefore provides in a further aspect pharmaceutical compositions comprising a compound of Formula 1 or a pharmaceutically acceptable salt thereof and a pharmaceutically acceptable carrier. Such compositions include those suitable for oral, parenteral or rectal administration.

PHARMACEUTICAL COMPOSITIONS

Compounds of Formula 1 and their pharmaceutically acceptable salts which are active when given orally can be formulated as liquids for example syrups, 5 suspensions or emulsions, tablets, capsules and lozenges.

A liquid composition will generally consist of a suspension or solution of the compound or pharmaceutically acceptable salt in a suitable liquid carrier(s), for example ethanol, glycerine, sorbitol, non-aqueous solvent such as polyethylene glycol, oils or water, with a suspending agent, preservative, surfactant, wetting agent, 10 flavoring or coloring agent. Alternatively, a liquid formulation can be prepared from a reconstitutable powder.

For example a powder containing active compound, suspending agent, sucrose and a sweetener can be reconstituted with water to form a suspension; and a syrup can be prepared from a powder containing active ingredient, sucrose and a sweetener.

A composition in the form of a tablet can be prepared using any suitable pharmaceutical carrier(s) routinely used for preparing solid compositions. Examples of such carriers include magnesium stearate, starch, lactose, sucrose, microcrystalline cellulose and binders, for example polyvinylpyrrolidone. The tablet can also be provided with a color film coating, or color included as part of the carrier(s). In 20 addition, active compound can be formulated in a controlled release dosage form as a tablet comprising a hydrophilic or hydrophobic matrix.

A composition in the form of a capsule can be prepared using routine encapsulation procedures, for example by incorporation of active compound and excipients into a hard gelatin capsule. Alternatively, a semi-solid matrix of active compound and high molecular weight polyethylene glycol can be prepared and filled into a hard gelatin capsule; or a solution of active compound in polyethylene glycol or a suspension in edible oil, for example liquid paraffin or fractionated coconut oil can be prepared and filled into a soft gelatin capsule. Compound of Formula 1 and their pharmaceutically acceptable salts which are active when given parenterally can be 30 formulated for intramuscular or intravenous administration.

A typical composition for intra-muscular administration will consist of a suspension or solution of active ingredient in an oil, for example arachis oil or sesame oil. A typical composition for intravenous administration will consist of a sterile isotonic aqueous solution containing, for example active ingredient, dextrose, sodium

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chloride, a co-solvent, for example polyethylene glycol and, optionally, a chelating agent, for example ethylenediamine tetracetic acid and an anti-oxidant, for example, sodium metabisulphite. Alternatively, the solution can be freeze dried and then reconstituted with a suitable solvent just prior to administration.

Compounds of structure (1) and their pharmaceutically acceptable salts which are active on rectal administration can be formulated as suppositories. A typical suppository formulation will generally consist of active ingredient with a binding and/or lubricating agent such as a gelatin or cocoa butter or other low melting vegetable or synthetic wax or fat.

Compounds of Formula 1 and their pharmaceutically acceptable salts which are active on topical administration can be formulated as transdermal compositions. Such compositions include, for example, a backing, active compound reservoir, a control membrane, liner and contact adhesive.

The typical daily dose of a compound of Formula 1 varies according to 15 individual needs, the condition to be treated and with the route of administration. Suitable doses are in the general range of from 0.001 to 10 mg/kg bodyweight of the recipient per day.

Within this general dosage range, doses can be chosen at which the compounds of Formula 1 lower plasma cholesterol levels and raise metabolic rate 20 with little or no direct effect on the heart. In general, but not exclusively, such doses will be in the range of from lower doese (0.001 to 0.5 mg/kg) to higher doses (0.5 to 10 mg/kg).

In addition, within the general dose range, doses can be chosen at which the compounds of Formula 1 lower plasma cholesterol levels and have little or no effect 25 on the heart without raising metabolic rate. In general, but not exclusively, such doses will be in the range of from 0.001 to 0.5 mg/kg.

It is to be understood that the 2 sub ranges noted above are not mutually exclusive and that the particular activity encountered at a particular dose will depend on the nature of the compound of Formula 1 used.

Preferably, the compound of Formula 1 is in unit dosage form, for example, a tablet or a capsule so that the patient may self-administer a single dose. In general, unit doses contain in the range of from 0.05-100 mg of a compound of Formula 1. Preferred unit doses contain from 0.05 to 10 mg of a compound of Formula 1.

The active ingredient may be administered from 1 to 6 times a day. Thus daily doses are in general in the range of from 0.05 to 600 mg per day. Preferably, daily doses are in the range of from 0.05 to 100 mg per day. Most preferably from 0.05 to 5 mg per day.

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EXAMPLES

EXAMPLE 1 - SYNTHESIS OF TR LIGANDS

Many TR ligands are known in the art, including T4 (thyroxine), T3, T2 and TS-9. See Jorgensen, Thyroid Hormones and Analogs, in *Hormonal Proteins and* 10 *Peptides, Thyroid Hormones* 107-204 (Choh Hao Li ed., 1978), incorporated by reference herein.

The syntheses of several TR ligands are described below.

Synthesis of TS1, TS2, TS3, TS4, TS5

TS1, TS2, TS3, TS4 and TS5 and analogs thereof can all be prepared by simple acylation of the nitrogen atom of any thyronine analog, including T3 (3,5,3'-triiodo-L-thyronine), T4 (thyroxine) and 3,5-diiodothyronine. TS1 and TS2 are synthesized by reacting T3 with Ph₂CHCO₂NHS (N-hydroxy succinimide-2,2-diphenylacetate) and C₁₆H₃₃CO₂NHS, respectively. TS3 is synthesized by reacting T3 with FMOC-Cl (fluorenylmethyloxycarbonylchloride). TS4 is synthesized by reacting T3 with tBOC₂O (tBOC anhydride or di-t-butyldicarbonate). TS5, which differs from TS1-4 by having a -H instead of an -I at the R'₃ position, is synthesized by reacting 3,5-diiodothyronine with tBOC₂O. The general reaction scheme for TS1, TS2, TS3, TS4 and TS5 is depicted in FIG. 11. It should be noted that in the reaction scheme, both TS5 and its precursor both have a hydrogen rather than an iodine at the R'₃ position.

Synthesis of TS6 and TS7

TS6 is synthesized by reacting TS5 with paranitrophenylisocyanate. TS7 is synthesized by reacting TS6 with TFA (trifluoroacetic acid), which cleaves the tBOC group. These reactions are simple organic synthesis reactions that can be performed by anyone of ordinary skill in the art. The synthetic scheme for TS6 and TS7 is diagrammed in **FIG. 12**.

Synthesis of TS8

TS8 is synthesized by reacting TS5 with Ph₂CHNH₂ (diphenylmethylamine) in the presence of triethylamine and any amide forming condensing reagent, such as 5 TBTU (hydroxybenztriazoleuronium tetrafluoroborate) or HBTU (hydroxybenztriazoleuronium hexafluorophosphate). The synthesis scheme for TS8 is depicted in FIG. 13.

SYNTHESIS OF 3,5-DIIODO-3'ISOPROPYLTHYRONINE DERIVATIVES

For designing a class of antagonists, it is important to have a hydrophobic group at the 3' position as well as an extension at the 5' position. Preferred hydrophobic groups at the 3' position include: methyl, benzyl, phenyl, iodo, and heterocyclic structures. The synthesis of a 3,5-diiodo-3'-isopropyl-5'-substituted thyronine is described below. The example provided describes the specific steps for synthesizing the TS10 compound, but this general reaction scheme can be used by one of ordinary skill in the art to synthesize any number of 3,5,-diiodo-3'-isopropyl-5'-substituted thyronine derivatives, which are characterized by having an extension at the 5' position. Additional compounds of this class can be synthesized using known organic synthesis techniques.

The synthesis of TS10 is described below and is depicted in FIG. 14. Numbers used in the reaction scheme for TS10 indicating the reaction product for each step are in parentheses.

2-Formyl-6-isopropylanisole (1): 2-formyl-6-isopropylanisole (10.0 g, 61 mmol), as made by Casiraghi, *et al.* JCS Perkin I, 1862 (1980) (incorporated by reference), is added dropwise to a suspension of sodium hydride (3.7 g, 153 mmol) in 50 mL THF and 50 mL of DMF in a round bottom flask. The addition generates an exothermic reaction and formation of a gray solid. Methyl iodide (26.0 g, 183 mmol) is then added dropwise and the reaction mixture is stirred at room temperature for 5 hours. The reaction mixture is quenched with 20 mL of water, then poured into 500 mL of water, and is extracted with ether (2 x 300 mL). The ether layers are combined, washed with water (5 x 1000 mL), dried over magnesium sulfate and concentrated in vacuo to provide 10.2 g (94%) of the title compound, with the following ¹H NMR (CDCl₃) properties: d 10.30 (s, 1H), 7.63 (d, 1H, J=3 Hz), 7.50

(d, 1H, J=3 Hz), 7.13 (t, 1H, J=3 Hz), 3.81 (s, 3H), 3.31 (heptet, 1H, J=7.5 Hz), 1.19 (d, 6H, J=7.5 Hz).

2-(2-Hydroxynonyl)-6-isopropylanisole (not shown in scheme):

5 Octylmagnesium chloride (8.4 mL, 16.9 mmol, 2.0 M) is added dropwise to a solution of 1 (1.5 g, 8.4 mmol) in 10 mL THF at -78°C. The reaction mixture is stirred for 2 hours with warming to room temperature. The reaction mixture is diluted with 50 mL ether and poured into 50 mL water. The ether layer is washed with brine (1 x 50 mL), dried over sodium sulfate, and concentrated in vacuo. Flash chromatography (silica 10 gel, 10% ether/hexane → 15% ether/hexane) provides 734 mg (30%) of the title compound with the following ¹H NMR (CDCl₃) properties: d 7.33-7.10 (m, 3H), 5.00 (br. s, 1H), 3.81 (s, 3H), 3.33 (heptet, 1H, J=7 Hz) 1.90-1.19 (m, 14H), 0.86 (t, 3H, J=6.5 Hz); HRMS (EI), found: 292.2404; calc'd: 292.2402.

2-nonyl-6-isopropylanisole (2): Compound 2 (663 mg, 2.3 mmol) is dissolved in solution of 5 mL ethanol and 5 mL acetic acid, and a spatula tip of palladium on carbon catalyst is added. The reaction mixture is then charged with hydrogen gas (using a simple balloon and needle) and the mixture is stirred at room temperature overnight. The next day, the reaction mixture is poured into ether (100 mL) and the ether layer is extracted with saturated sodium bicarbonate (3 x 100 mL). The ether layer is dried over sodium sulfate and concentrated *in vacuo* to provide 581 mg (91%) of (2) with the following ¹H NMR (CDCl₃) properties: d 7.14-7.00 (m, 3H), 3.75 (s, 3H), 3.36 (heptet, 1H, J=6.8 Hz), 2.63 (t, 2H, J=7.5 Hz), 1.68-1.15 (m, 14H), 0.86 (t, 3H, J=5.5 Hz); HRMS (EI), mass found: 276.2459; calculated: 276.2453.

Thyronine adduct (4): Fuming nitric acid (0.071 mL) is added to 0.184 mL acetic anhydride chilled to -5°C. Iodine (66 mg) is added to this mixture followed by trifluoroacetic acid (0.124 mL). This mixture is stirred for 1 hour with warming to room temperature, at which point all of the iodine is dissolved. The reaction mixture was then concentrated *in vacuo* to provide an oily semi-solid material. The residue was dissolved in 0.7 mL of acetic anhydride and cooled to -20°C. A solution of anisole (2) (581 mg, 2.1 mmol) in 1.2 mL acetic anhydride and 0.58 mL TFA is added dropwise. The reaction mixture is stirred at -20° for 1 hour, then stirred overnight with warming to room temperature. The reaction mixture is partitioned between water and methylene chloride. The methylene chloride layer is dried over sodium

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sulfate and concentrated *in vacuo* to provide the iodonium salt (3) as an oil. This material is not purified or characterized, and is directly introduced into the coupling reaction.

N-Trifluoroacetyl-3,5-diiodotyrosine methyl ester (552 mg, 1.0 mmol) prepared according to the procedure of N. Lewis and P. Wallbank, *Synthesis* 1103 (1987) (incorporated by reference) and all of the crude iodonium salt (3) from above is dissolved in 5 mL of anhydrous methanol. Diazabicyclo[5.4.0]undecane (DBU) (183 mg, 1.2 mmol) and a spatula tip of copper-bronze are added and the resulting mixture is stirred at room temperature overnight. The next day, the reaction mixture is filtered, and the filtrate is concentrated *in vacuo*. The crude residue is purified by flash chromatography (silica gel, 10% ethyl acetate/hexane) to provide 30 mg (4%) of the protected thyronine adduct (4).

Deprotected thyronine (TS10): The protected thyronine 4 (30 mg, 0.04 mmol) is dissolved in a mixture of 2.25 mL acetic acid and 2.25 mL 49% hydrobromic acid.

15 The reaction mixture is heated to reflux for 5 hours. The reaction mixture is cooled to room temperature, and the solvents are removed *in vacuo*. Water is added to triturate the oily residue into a gray solid. This solid material is filtered, washed with water, and dried over P₂O₅ *in vacuo* to provide 24 mg (81%) of the title compound, TS10, with the following ¹H NMR (CDCl₃) properties: d 7.57 (s, 1H), 6.86 (s, 1H), 6.45 (s, 20 1H), 6.34 (s, 1H), 4.81 (m, 1H), 3.86 (s, 3H), 3.71 (s, 3H), 3.33-3.05 (m, 3H), 2.58-2.47 (m, 2H), 1.62-0.76 (m, 23H); MS (LSIMS): M⁺ = 817.0.

As mentioned above, this reaction scheme can be modified by one of ordinary skill in the art to synthesize a class of compounds characterized by 3,5-diiodo-3'isopropylthyronine derivatives, wherein (1) the 3' isopropyl group can be replaced with a hydrophobic group, including methyl, benzyl, phenyl, iodo, and heterocyclic structures, and (2) a wide variety of chemical structures can be incorporated at the 5' position, including alkyl groups, planar aryl, heterocyclic groups, or polar and/or charged groups.

The aldehyde (1) in the above reaction scheme is a versatile synthetic 30 intermediate which allows for the attachment of a variety of chemical moieties to the 5' position of the final thyronine derivative. In addition, a variety of chemical reactions can be used to attach the chemical moieties. These reactions are well known in the art and include organometallic additions to the aldehyde (including Grignard reagents, organolithiums, etc.), reductive amination reactions of the aldehyde with a

primary or secondary amine, and Wittig olefination reactions with a phosphorous ylid or stabilized phosphonate anion. Other possibilities include reduction of the aldehyde to a benzyl alcohol allowing for etherification reactions at the 5' position. As mentioned above, these methods allow for a wide variety of chemical structures to be incorporated at the 5' position of the final thyronine derivative, including alkyl groups, planar aryl, heterocyclic groups or polar and/or charged groups.

Synthesis of 3, 5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy) benzoic acid (Compound 11).

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- (a) A mixture of 2,6-diisopropyl phenol (20 g, 0.11 mol), potassium carbonate (62 g, 0.45 mol), acetone (160 ml) and methyl iodide (28 ml, 0.45 mole) is refluxed for three days. The reaction mixture is filtered through celite, evaporated, dissolved in ether, washed twice with 1M sodium hydroxide, dried over magnesium sulphate and concentrated to afford 15.1 g (0.08 mol, 70%) of 2,6-diisopropyl anisole as a 20 slightly yellow oil.
- (b) Fuming nitric acid (12.4 ml, 265 mmol) is added dropwise to 31.4 ml of acetic anhydride which is cooled in a dry ice/carbon tetrachloride bath. Iodine 11.3 g, 44.4 mmol) is added in one portion followed by dropwise addition of trifluoroacetic acid (20.5 ml, 266 mmole). The reaction mixture is stirred at room temperature until all the iodine is dissolved. Nitrogen oxides are removed by flushing nitrogen into the vessel. The reaction mixture is concentrated, the residue is dissolved in 126 ml of acetic anhydride and is cooled in a dry ice/carbon tetrachloride bath. To the stirred solution 2,6-diisopropylanisole (51 g, 266 mmol) in 150 ml of acetic anhydride and 22.6 ml of trifluoroacetic acid is added dropwise. The reaction mixture is left to stand at room temperature over night and then is concentrated. The residue is taken up in 150 ml of methanol and treated with 150 ml of 10% aqueous sodium bisulfite solution and 1 liter of 2M sodium borotetrafluoride solution. After the precipitate aggregates, petroleum ether is added and the supernatant is decanted. The precipitate is triturated with petroleum ether, filtered, washed with petroleum ether and dried at room

temperature in vacuo. This affords 34 g (57 mmol, 65%) of bis(3,5-diisopropyl-4-methoxyphenyl)iodonium tetrafluoroborate as a white solid.

- (c) To a stirred solution of 3,5-dibromo-4-hydroxybenzoic acid (12 g, 40.5 mmol) in 250 ml of methanol, thionyl chloride (3 ml) is added dropwise. The 5 reaction mixture is refluxed for five days, water is added and the precipitated product is filtered off. The residue is dissolved in ethyl acetate. From the aqueous phase, methanol is removed by concentration. The aqueous phase is then saturated with sodium chloride, and extracted with ethyl acetate. The combined organic phases are dried over magnesium sulphate, filtered and concentrated. This gives 12.5 g (40.5 mmol, 100%) of 3,5-dibromo-4-hydroxymethyl benzoate as a white crystalline solid.
- (d) The products obtained in steps b and c are reacted with each other according to the following protocol. To bis(3,5-diisopropyl-4-methoxyphenyl)iodonium tetrafluoroborate (2.86 g, 4.8 mmole) and copper bronze (0.42 g, 6.4 mmole) in 7 ml. of dichloromethane at 0°C is added dropwise a solution of 3,5-dibromo-4-hydroxymethyl benzoate (1.0 g, 3.2 mmole) and triethylamine (0.36 g, 3.5 mmole) in 5 ml of dichloromethane. The reaction mixture is stirred in the dark for eight days and then is filtered through celite. The filtrate is concentrated and the residue is purified by column chromatography (silica gel, 97:3 petroleum ether/ethyl acetate) to give 0.62 g (1.2 mmole, 39%) of 3,5-dibromo-4-(3',5'-diisopropyl-4'-20 methoxyphenoxy)methyl benzoate as a solid.
- The product from step d (0.2 g, 0.4 mmole) is dissolved in 2 ml. dichloromethane, is put under nitrogen and is cooled at -40°C. To the stirred solution is added 1M BBr₃ (1.2 ml, 1.2 mmole) dropwise. The reaction mixture is allowed to reach room temperature and then is left over night. It is cooled to 0°C and then 25 hydrolyzed with water. Dichloromethane is removed by concentration and the aqueous phase is extracted with ethyl acetate. The organic phase is washed with 1M hydrochloric acid and brine. Then it is dried over magnesium sulphate, filtered and concentrated. The residue is chromatographed (silica, 96:3.6:0.4 dichloromethane/methanol/acetic acid) producing 93 mg (0.2 mmole, 51%) of 3,5-30 dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy)benzoic acid as a white solid. ¹H nmr (CDCl₃) δ 1.23 (d, 12H, methyl), 3.11 (m, 2H, CH), 6.50 (s, 2H, 2,6-H) 8.33 (s, 2H, 2',6'-H).

Synthesis of addition ligands are described in U.S. Serial No. 08/877,792, filed June 18, 1997 which is herein incorporated in its entirety by reference.

TABLE 2 and **FIG. 15** depict the structures of several TR ligands in reference to Formula I.

5

TABLE 2

Cmpd	R ₃	R,	R ₅	R'3	R',	R's	R ₁
*T ₃	-1	-0-	-I	-I	-OH	-H	-CH ₂ CH(NH ₂)CO ₂ H
*T ₄	-I	- O-	-I	-I	-OH	-I	-CH₂CH(NH₂)CO₂H
TS1	-l	-0-	-I	-l	-OH	-H	-CH₂CH[NHCOCH∮₂]CO₂H
TS2	I-	-0-	-1	-I	-OH	-Н	-CH ₂ CH[NHCO(CH ₂) ₁₅ CH ₃]CO ₂ H
TS3	-I	-0-	-1	-1	-ОН	-H	-CH2CH[NH-FMOC]CO2H
TS4	-1	-0-	-1	-i	-ОН	-H	-CH₂CH[NH-tBOC]CO₂H
TS5	-I	-0-	-I	-H	-OH	-H	-CH₂CH[NH-tBOC]CO₂H
TS6	-J	-0-	-I	-H	-OC(O)NH=Ø _p NO ₂	-H	-CH₂CH[NH-tBOC]CO₂H
TS7	-I	-0-	- I	-1	- OC(O)NH=NHØNO₂	-H	-CH₂CH(NH₂)CO₂H
TS8	J	-0-	-1	-H	-NH-CHØØ	-Н	-CH₂CH[NH-tBOC]CO₂H
TS9	-I	-0-	I-	-IsoPr	-OH	-Н	-CH₂CH(NH₂)CO₂H
TS10	-I	-0-	-I	-IsoPr	-ОН	-(CH) ₈ - CH ₃	-CH₂CH(NH₂)CO₂H

*

Prior Art Compound

-Ø:

phenyl

-ØpNO₂:

para nitro phenyl

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EXAMPLE 2 - RECEPTOR BINDING ASSAYS OF TR LIGANDS

To test the ability of synthesized TR ligands to bind to a thyroid receptor (TR), the binding affinity of a TR ligand for TR is assayed using TR's prepared from rat liver nuclei and [125]T₃ as described in J.D. Apriletti, J.B. Baxter, and T.N. Lavin, J. 15 Biol. Chem., 263: 9409-9417 (1988). The apparent Kd's are calculated using the method described by Apriletti (1995) and Apriletti (1988). The apparent Kd's are presented in TABLE 3. The apparent Kd's (App.Kd) are determined in the presence

of the sample to be assayed, 1 nM [¹²⁵I]T₃, and 50Tg/ml core histones, in buffer E (400 mM KCl, 200 mM potassium phosphate, pH 8.0, 0.5 mM EDTA, 1 mM MgCl₂, 10% glycerol, 1 mM DTT) in a volume of 0.21 ml. After incubation overnight at 4°C, 0.2 ml of the incubation mixture is loaded onto a Quick-Sep Sephadex G-25 column 5 (2.7 x 0.9 cm, 1.7 ml bed volume) equilibrated with buffer E. The excluded peak of protein-bound [¹²⁵I]T₃ is eluted with 1 ml of buffer E, collected in a test tube, and counted. Specific T₃ binding is calculated by subtracting nonspecific binding from total binding.

TABLE 3

Compound	App.Kd(nM)	Coactivation Assay RIP-140	EC ₅₀ (M)
T ₃	0.06	+	10-10
T ₄	2	+	10-9
TS1	4	+	10-7
TS2	1400	nd	nd
TS3	4	+ .	10 ⁻⁸
TS4	8	+	nd
TS5	. 220	+	10-6
TS6	>10000	nd	nd
TS7	260	+	10-7
TS8	6000	nd	nd
TS9	1	+	10-10
TS10	400	+	10-6

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+: RIP-140 Binding

-: RIP-140 Binding

nd: Not Determined

EXAMPLE 3 - INCREASED NUCLEAR PROTEIN COACTIVATION BY TR LIGANDS

To test the ability of TR ligands to activate the binding of TR to the nuclear activation protein RIP-140 (a nuclear protein that can bind to nuclear receptors, such as the estrogen receptor), a TR ligand is liganded to TR and then incubated with RIP-140 as described in V. Cavailles, et al., EMBO J., 14(15):3741-3751 (1995), which is incorporated by reference herein. In this assay, ³⁵S-RIP-140 protein binds to liganded TR but not unliganded TR. Many TR ³⁵S ligands can activate RIP-140 binding as shown in **TABLE 3**.

10 Example 4 - TR Ligand binding and TR activation in Cultured Cells

To test TR activation of transcription in a cellular environment, TR ligands are assayed for their ability to activate a reporter gene, chloramphenicol transferase ("CAT"), which has a TR DNA binding sequence operatively linked to it. Either GC or L937 cells (available from the ATCC) can be used, respectively). In such assays, a 15 TR ligand crosses the cell membrane, binds to the TR, and activates the TR, which in turn activates gene transcription of the CAT by binding the TR DNA binding region upstream of the CAT gene. The effective concentration for half maximal gene activation (EC50) is determined by assaying CAT gene activation at various concentrations as described herein and in the literature. The results of CAT gene 20 activation experiments are shown in TABLE 3.

CAT GENE ACTIVATION ASSAYS

Functional response to thyroid hormone (3,5,3'-triiodo-L-thyronine, T₃) and TR ligands is assessed either in a rat pituitary cell line, GC cells, that contain endogenous thyroid hormone receptors (TRs) or U937 cells that contain exogenous TRs expressed as known in the art. GC cells are grown in 10-cm dishes in RPMI 1640 with 10% newborn bovine serum, 2 mM glutamine, 50 units/ml penicillin and 50 Tg/ml streptomycin. For transfections, cells are trypsinized, resuspended in buffer (PBS, 0.1% glucose) and mixed with a TREtkCAT plasmid (10 mg) or phage in 0.5 ml buffer (15±5 million cells) and electroporated using a Bio-Rad gene pulser at 0.33 kvolts and 960 mF. The TREtkCAT plasmid contains two copies of a T₃ response element (AGGTCAcaggAGGTCA) cloned in the Hind III site of the pUC19 polylinker immediately upstream of a minimal (-32/+45) thymidine kinase promoter

linked to CAT (tkCAT) coding sequences. After electroporation, cells are pooled in growth medium (RPMI with 10% charcoal-treated, hormone stripped, newborn bovine serum), plated in 6-well dishes and treated with either ethanol or hormone. CAT activity is determined 24 hours later as described D. C. Leitman, R. C. J. 8 Ribeiro, E. R. Mackow, J. D. Baxter, B. L. West, *J. Biol. Chem.* 266, 9343 (1991), which is incorporated by reference herein.

EFFECT OF TS-10 ON THE TRANSCRIPTIONAL REGULATION OF THE DR4-ALP REPORTER GENE IN THE PRESENCE OR ABSENCE OF T3.

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Characteristics of the TRAF cells: TRAFa1 are CHO K1 cells stably transformed with an expression vector encoding the human thyroid hormone receptor α1 and a DR4,ALP reporter vector; TRAFb1 are CHO K1 cells stably transformed with an expression vector encoding the human thyroid hormone receptor β1 and a 15 DR4-ALP reporter vector.

Interpretation of the effect of compound TS-10 on the transcriptional regulation of the DR4-ALP reporter gene in the presence or absence of T3.

TRAFa1 reporter cells: TS-10 alone (open circles) induces a partial activation of the expression of the ALP reporter protein amounting to approximately 27% of the maximal effect by the natural thyroid hormone T3. In the presence of T3 (filled circles), TS-10 has a weak antagonistic effect. The EC50 concentration for the agonistic effect of TS-10 and the EC50 concentration for its T3 antagonistic effect, 25 respectively, is indicated in FIG. 18.

In FIG. 18, open and filled circles with dotted lines show the dose-dependent effect of TS-10/T3 on the toxicity marker (MTS/PMS), reduction of tetrazolium salt in the mitochondria, displayed on the right y-axis as optical density. There is no 30 obvious toxic effect of TS-10 on the MTS-PMS marker but there is a clear effect on the morphology of the cells, as can be seen under the light microscope, at the highest concentration of TS-10 (32 mM) both in the absence and presence of T3, respectively (not shown in the figure).

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TRAFb1 reporter cells: TS-10 alone (open circles) induces a partial activation of the expression of the ALP reporter protein amounting to approximately 35% of the maximal effect by T3. The EC50 concentration for the agonistic effect of 5 TS-10 is indicated in FIG. 19. In the presence of T3 (filled circles), TS-10 shows, if anything, a slight potentiation of the T3 effect on the expression of the ALP reporter protein. The T3 inhibitory effect of TS-10 at its highest concentration used (32 mM) is a toxic effect rather than T3 antagonism.

In **FIG. 19**, open and filled circles with dotted lines show the dose-dependent effect of TS-10/T3 on the toxicity marker (MTS/PMS), reduction of tetrazolium salt in the mitochondria, displayed on the right y-axis as optical density. There is no obvious toxic effect of TS-10 on the MTS-PMS marker but a clear effect on the morphology of the cells can be observed, under the light microscope, at the highest concentration of TS-10 (32 mM) both in the absence and presence of T3, respectively (not shown in the figure).

HepG2 (HAF18) reporter cells: TS-10 alone (open circles) induces a partial activation of the expression of the ALP reporter protein amounting to slightly more 20 than 50% of the maximal effect by T3. The EC50 concentration for the agonistic effect of TS-10 is indicated in FIG. 20. In the presence of T3 (filled circles), TS-10 shows no effect i.e. no T3 antagonism nor potentiation/additive effect to T3. Open and filled circles with dotted lines show the dose-dependent effect of TS-10/T3 on the toxicity marker (MTS/PMS), reduction of tetrazolium salt in the mitochondria, 25 displayed on the right y-axis as optical density. There is no obvious toxic effect of TS-10 on the MTS/PMS marker or on the morphology of the cells, as can be observed using a light microscope, at any concentration of TS-10/T3 used.

Example 5 - Comparisons of Human TR- α and Human TR- β

Competition for $[^{125}I]T_3$ binding to TR LBD by T_3 and Triac

The drug, Triac, is a thyroid hormone agonist. Triac is 3,5,3'-triiodothyroacetic acid and is described in Jorgensen, Thyroid Hormones and Analogs in *Hormonal Proteins and Peptides, Thyroid Hormones* at 150-151 (1978). Another

compound that can be used in place of Triac is 3,5-diiodo-3'-isopropylthyroacetic acid. Competition assays are performed to compare the displacement of [¹²⁵I]T₃ from binding with human TR-α LBD or human TR-β LBD by unlabeled T₃ or Triac. The results of such assays are depicted in **FIG. 16**.

5 Standard binding reactions are prepared containing 1 nM [¹²⁵I]T₃, 30 fmol of human TR-α (empty symbols) or β (solid symbols), and various concentrations of competing unlabeled T₃ (circles) or Triac (triangles). Assays are performed in duplicate.

Competition for [125I]T₃ binding to variant TR LBD by T₃, Triac and GC-1

The following assays residues involved in selective binding among TR isoforms. Competition assays are performed to compare the displacement of [125]T] from binding with wild-type human TR-α LBD or human TR-β LBD, to a variant form of the TR LBDs by unlabeled T3, Triac or GC-1. A variant TR-α or TR-β is constructed by substituting an amino acid found in the corresponding position of the other TR isoform. For example, asparagine 331 in human TR-β corresponds to serine 277 in human TR-α. To test binding specificity contributed by this position, a variant human TR-β is constructed that contains asparagine 331 substituted with a serine residue (designated Asn331Ser or N331S). Binding assays are described in *Apriletti* 20 et al. (Protein Expression and Purification 6:363-370 (1995)). The results of such assays are depicted in FIG. 27, and summarized in Table 4 below.

TABLE 4	
Effect of TR-β Substitution N331S on Binding Affinity	,

Ligand	Native TR-α	Native TR-β	Mutant TR-β
T3	20 pM	60 pM	100 pM
T4	600	3000	ND
Triac	20	20	100
IpBr ₂	17	ND	ND
Dimit	6000	8000	ND
GC-1	200	40	400

Competition curves comparing wildtype TR-β versus the variant TR-β N331S for 5 binding T3, Triac or GC-1 show that the affinity of the mutant receptor for Triac was reduced to approximately the same as for T3 (vs. 3-fold greater in wild type) so that the relative affinities are similar to wild-type TR-α. The affinity for GC-1 was also reduced to several fold less than T3, as is seen with TR-α.

Comparison of the affinity of TR- β variant N331S to the native TRs for 10 selected ligands is as follows:

Native TR-α for various ligands (T3, T4, Triac, IpBr2, Dimit, GC-1):

 $IpBr_2$. > Triac \cong T3 > GC-1 > T4 > Dimit

Native TR-β (T3, T4, Triac, Dimit, GC-1)

Triac > GC-1 \geq T3 > T4 > Dimit

15 Variant TR-β (N331S) (T3, Triac, GC-1)

Triac \cong T3 > GC-1.

Scatchard Analysis of [125I]T₃ Binding to TR

Human TR- α (left panel) or human TR- β (right panel) is assayed for T₃ 20 binding in the presence of increasing concentrations of [^{125}I]T₃. The apparent equilibrium dissociation constant (20 pM for I and 67 pM for β) is calculated by linear regression analysis and is depicted in **FIG. 17**.

3, 5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy) Benzoic Acid is a TR- α Selective Synthetic Ligand.

3, 5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy) benzoic acid (Compound 11), the structure of which is drawn above, is assayed for binding to the two different isoforms of the TR, TR-α and TR-β. Compound 11 exhibits an IC50 of 1.6 TM for binding to TR-α and an IC50 of 0.91 TM for binding to TR-β. Assays for determining selective binding to the TR-α or TR-β LBD can include reporter assays, 15 as described herein. See also Hollenberg, et al., J. Biol. Chem., (1995) 270(24):14274-14280.

Example 6 - Preparation and Purification of a $TR-\alpha$ LBD

Rat TR-α LBD, residues Met122 - Val410, is purified from *E. coli* ("LBD-20 122/410"). The expression vector encoding the rat TR-α LBD is freshly transfected into *E. coli* strain BL21(DE3) and grown at 22°C in a 50-liter fermenter using 2x LB medium. At an A₆₀₀ of 2.5-3, IPTG is added to 0.5 mM and growth is continued for 3 h before harvesting. The bacterial pellet is quickly frozen in liquid nitrogen and stored at -70°C until processed. Extraction and purification steps are carried out at 25 4°C. The bacteria are thawed in extraction buffer (20MM Hepes, pH 8.-, 1 mM EDTA, 0.1% MTG, 0.1 mM PMSF, and 10% glycerol) at a ratio of 10 ml buffer/g bacteria. Bacteria are lysed by incubation for 15 min. with 0.2 mg/ml lysozyme and sonicated at maximum power while simultaneously homogenized with a Brinkmann homogenizer (Model PT 10/35 with generator PTA 35/2) until the solution loses its 30 viscosity. After centrifugation for 10 min at 10,000 g, the supernatant is adjusted to 0.4 M KCl, treated with 0.6% PEI to precipitate fragmented DNA, and centrifuged for 10 min at 10,000 g. The rat TR-α LBD in the supernatant is then precipitated with 50% ammonium sulfate and centrifuged for 10 min at 10,000 g. The precipitate is

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resuspended with buffer B (20 mM Hepes, pH 8.0, 1 mM EDTA, 1 mM DTT, 0.1 mM PMSF, 0.01% Lubrol, and 10% glycerol) to a final conductivity of 9 mS/cm (approx. 0.7 M ammonium sulfate) and centrifuged 1 h at 100,000g. The supernatant is frozen in liquid nitrogen and stored at -70°C.

The crude extract is thawed, bound with a tracer amount of [125I]T3, and loaded directly onto a phenyl-Toyopearl hydrophobic interaction column (2.6 x 18 cm, 95 ml bed volume) at 1.5 ml/min. The column is eluted with a 2-h gradient from 0.7 ammonium sulfate, no glycerol to no salt, 20% glycerol in buffer C (20 mM Hepes, pH 8.0, 0.5 mM EDTA, 1 mM DTT, 0.2 mM PMSF). The rat TR-α LBD 10 prebound to tracer [125I]T₃ (less than 0.005% of total rat TR-α LBD) is detected using a flow-through gamma emission detector, whereas unliganded rat TR-I LBD is assayed by postcolumn [125I]T₃ binding assays (described herein).

The phenyl-Toyopearl unliganded rat TR-α LBD peak fractions are pooled, diluted with buffer B to a conductivity of 0.5 mS/cm (equivalent to approx. 20 mM 15 ammonium sulfate), loaded onto a TSK-DEAE anion-exchange column (2 x 15 cm, 47 ml bed volume) at 4 ml/min, and eluted with a 60-min gradient from 50 to 200 mM NaCl in buffer B.

The unliganded rat TR-\alpha LBD peak fractions from TSK-DEAE are pooled, diluted twofold with buffer B, loaded at 0.75 ml/min on a TSK-heparin HPLC column 20 (0.8 x 7.5 cm, 3 ml bed volume), and eluted with a 50 to 400 mM NaCl gradient in buffer B.

The pool of unliganded rat TR-α LBD peak fractions from the TSK-heparin column is adjusted to 0.7 M ammonium sulfate, loaded at 0.75 ml/min on a TSKphenyl HPLC column (0.8 x 7.5 cm, 3 ml bed volume), and eluted with a 60-min 25 gradient from 0.7 M ammonium sulfate without glycerol to no salt with 20% glycerol in buffer C. The fractions containing unliganded rat TR-α LBD are pooled and incubated with a five fold excess of hormone for 1 h, the salt concentration is adjusted to 0.7 M ammonium sulfate, and the sample is reloaded and chromatographed on the same column as described above.

Example 7 - Crystallization of Liganded TR-α LBD

Material from a single LBD-122/410 preparation is divided into batches, and quantitatively bound with one of the following ligands: Dimit, T₃, or Triac IpBr₂ (3,5dibromo-3'isopropylthyronine) for the final purification step.

To maintain full saturation of rat TR-α LBD with a ligand, and to prepare the complex for crystallization, the ligand-bound rat TR-α LBD is concentrated and desalted in an Amicon Centricon-10 microconcentrator (McGrath et al, *Biotechniques*, (1989) 7:246-247, incorporated by reference herein), using 10 mM Hepes (pH 7.0), 3.0 mM DTT, and 1.0 nM to 10 nM ligand.

10 Factorial crystallization screening trials (Jancarik & Kim, J. Appl. Crystallogr. (1991) 24:409-411, incorporated by reference herein) are carried out for rat TR- α LBD bound to selected ligands using hanging-drop vapor diffusion at 17°C (with 1 µl protein solution, 1 µl precipitant solution and a 0.5 ml reservoir using silanized coverslip: (McPherson, Preparation and Analysis of Protein Crystals (1982), 15 incorporated by reference herein). Rat $TR-\alpha$ LBD is not stable at 4°C and is stored at -80°C, where it maintains its avidity for hormone and its crystallizability for approximately two to three months. These procedures are carried out as described in McGrath, M.E. et al., J. Mol. Biol. (1994) 237:236-239 (incorporated by reference). Crystals are obtained in condition 21 of the screening trials (Jancarik & Kim 1991) 20 and conditions are then optimized. Wedge-shaped crystals are reproducibly obtained with hanging-drop vapor fusion at 22°C with 15% 2-methyl-2,4-pentanediol (MPD), 0.2 M ammonium acetate and 0.1 M sodium cacodylate (pH 6.7), 3 mM DTT, with 2 μl protein solution, 1 μl precipitant solution and a 0.6 ml reservoir using silanized coverslip, and with 8.7 mg/ml (Dimit), 5.5 mg/ml (IpBr₂), 5 mg/ml (Triac), or 2.3 25 mg/ml (T₃) over a period of three days. Under these conditions, diffraction quality crystals (dimension 0.5 x 0.2 x 0.0075 mm³) can be grown at ambient temperature (22°C). The best crystals have a limiting dimension of approximately 100 Tm and are obtained at a protein concentration between 2.3 and 8.7 mg/ml in the presence of 3 mM DTT. The crystals are of the monoclinic space group C2, with one monomer in 30 the asymmetric unit.

Example 8 - Crystallization of Human TR- β LBD Complexed with T3, Triac, or GC-1

Human TR-β LBD complexed with T₃, Triac, or GC-1 are purified according to the same procedures described above for the rat TR-α LBD, with the following 5 modifications.

The expression of human TR-β LBD differs from the rat TR-α LBD in that the human TR-β LBD residues extend from the amino acid at position 716 through the amino acid at position 1022, according to the amino acid numbering scheme for the various nuclear receptor LBDs depicted in FIG. 3. FIG. 3 illustrates a numbering scheme applicable to all of the nuclear receptors listed as well as to any additional homologous nuclear receptors. The vertical lines on FIG. 3 at position 725 and at position 1025 delineate the preferred minimum amino acid sequence necessary to obtain adequate binding of ligand. The amino acid sequence from position 716 to position 1022 according to the numbering scheme of FIG. 3 corresponds to the amino 15 acid positions 202 to 461 according to the conventional numbering of the amino acid sequence of human TR-β which is publicly available. Also, the human TR-β LBD is expressed with a histidine tag, as described in Crowe *et al.*, *Methods in Molecular Biology* (1994) 31:371-387, incorporated by reference herein.

The purification of human TR-β LBD is the same as that described above for 20 the rat TR-α LBD with the following exceptions. First, before the purification step using the hydrophobic interaction column, a step is added in which the expressed human TR-β LBD is purified using a nickel NTA column (commercially available from Qiagen, Chatsworth, CA) according to manufacturer's instructions, and eluted with 200 mM imidazole. The second difference is that in the purification of the 25 human TR-β LBD, the purification step using a heparin column is omitted.

The crystallization of human TR-β LBD bound to T₃, Triac or GC-1 is as follows. Crystals are obtained in condition 7 of the factorial screen using hanging drops as before at ambient temperature (22°C) using the factorial crystallization screening trials of Jancarik & Kim (1991) and using the commercially available 30 product from Hampton Research, Riverside). The following are optimum conditions: hexagonal bipyrimidal crystals are grown at 4°C for 2-3 days from hanging drops containing 1.0-1.2 M sodium acetate (pH unadjusted) and 0.1 M sodium cacodylate (pH 7.4), 3 mM DTT, with either a 1 μl protein solution, 1 μl precipitant solution or 2

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μl protein solution, l μl precipitant solution and a 0.6 ml reservoir using silanized coverslip, at a protein concentration of 7-10 mg/ml. The best crystals have a limiting dimension of 200 µm. The following are optimum conditions for crystallization of the TR-β LBD with GC-1: hexagonal bipyrimidal crystals are grown at 4°C for 2-3 5 days from hanging drops containing 0.8-1.0M sodium acetate (pH unadjusted), 50-200nM sodium succinate, and 0.1M sodium cacodylate (pH 7.2), 3mM DTT, 1 µl protein solution, 1 µl precipitant solution and a 0.6ml reservoir using silanized coverslip, at a protein concentration of 7-10 mg/ml. The best crystals have a limiting dimension of 200 µM. The unit cell dimensions are cell length a=b=68.73, cell length 10 c=130.09. The unit cell angles are α =90°, β =90°, γ =120°.

The crystal system for human TR-β LBD bound to T₃, Triac or GC-1 is trigonal with the space group $p_{31}21$. The unit cell dimensions are cell length a = cell length b = 68.448 angstroms, cell length c = 130.559 angstroms. The angles are α = 90°, $\beta = 90°$, gamma = 120°.

15

Example 9 - Determination of Liganded TR-α LBD and TR-β Crystal **STRUCTURES**

Data from each cocrystal (Rat TR-a LBD with Dimit, T3 and IpBr2; Human TR-B LBD with Triac and GC-1) is measured on a Mar area detector at Stanford 20 Synchrotron Radiation Laboratory beamline 7-1 ($\lambda = 1.08$ angstroms) using 1.2° oscillations. Data from the cocrystal of the hTR-\$\beta\$ LBD with Triac is measured on a Mar area detector at Stanford Synchrotron Radiations Laboratory beamline 7-1 (λ = 1.08 angstroms) using 1.0 oscillations. Data from the cocrystal of the hTR-β LBd with GC-1 is measured on a R-axis II area detector on a Rigaku rotating Cu anode 25 (50kV, 300mA). The crystals are transferred into a cryosolvent containing 1.2M sodium acetate, 0.1M sodium cacodylate, adn 15% glycerol followed by a second transfer into 30% glycerol, then flash frozen in liquid nitrogen. An orientation matrix for each crystal is obtained using DENZO. The reflections are integrated with DENZO (commercially available from Molecular Structure Corp., The Woodlands, 30 Texas) and are scaled with SCALEPACK (as described in Otwinowski, Z, Proceedings of the CCP4 Study Weekend: "Data Collection and Processing," 56-62 (SERC Daresbury Laboratory, Warrington, UK 1993) incorporated by reference).

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For rTR-α cocrystals, data from the T₃ cocrystal is measured with the b* axis approximately parallel with the spindle. The crystals are flash frozen at -178°C in a nitrogen gas stream with the MPD mother liquor serving as the cryosolvent. An orientation matrix for each crystal is determined using REFIX (Kabsch, W., J. Appl. 5 Crystallogr. (1993) 26:795-800 incorporated by reference). Reflections are integrated with DENZO, and are scaled with SCALEPACK.

For the T₃ data set, Bijvoet pairs are kept separate, and are locally scaled using MADSYS (W. Hendrickson (Columbia University) and W. Weis (Stanford University)).

10 Cocrystals prepared from the three isosteric ligands are isomorphous. MIR analysis is performed using programs from the CCP4 suite (Collaborative Computational Project, N.R. Acta Crystallogr. (1994) D50:760-763, incorporated by reference herein). Difference Pattersons is calculated for both T₃ and IpBr₂, taking the Dimit cocrystal as the parent. The positions of the three iodine atoms in the T₃ 15 difference Patterson are unambiguously determined from the Harker section of the density map as peaks of 11[above background. The positions for the two bromine atoms in the IpBr2 cocrystals, are located independently, as peaks 8[above the noise level. Phases for the LBD-122/410 are calculated from the solution to the IpBr₂ difference Patterson, and are used to confirm the location of the unique third iodine of 20 the T₃ cocrystal. Halogen positions are refined with MLPHARE, including the anomalous contributions from the iodine atoms (Otwinowski, Z, Proceedings of the CCPR Study Weekend 80-86 (SERC Daresbury Laboratory, Warrington, UK 1991)). The MIRAS phases are improved through solvent flattening/histogram matching using DM (Cowtan, K., Joint CCP4 and ESF-EACBM Newsletter on Protein 25 Crystallography (1994) 31: 34-38, incorporated by reference herein).

A model of the LBD-122/410 with Dimit bound is built with the program O from the solvent flattened MIRAS 2.5 angstrom electron density map (Jones *et al.*, *Acta Crystallogr*. (1991) A 47:110-119, incorporated by reference herein). The initial model, without ligand, (Rcryst = 40.1%), is refined using least-squares protocols with XPLOR. The Dimit ligand is built into unambiguous Fo-Fc difference density during the following round. Subsequent refinement employs both least-squares and simulated annealing protocols with XPLOR (Brunger *et al.*, *Science* (1987) 235:458-460), incorporated by reference herein). Individual atomic B-factors are refined

isotropically. As defined in PROCHECK, all residues are in allowed main-chain torsion angle regions as described in Laskowski *et al.*, *J. Appl. Crystallogr.*, (1993) 26:283-291, incorporated by reference herein. The current model is missing 34 residues (Met₁₂₂-Gln₁₅₆) at the N-terminus, and 5 residues (Glu₄₀₆-Val₄₁₀) at the C-5 terminus.

In addition, the following residues are not modeled beyond Cβ due to poor density: 184, 186, 190, 198, 206, 209, 240, 301, 330, 337, 340, 343, 359, and 395. The average B-value for protein atoms is 34.5 Å². The final model consists of the LBD-122/410, residues Arg₁₅₇-Ser₁₈₃, Trp₁₈₅-Gly₁₉₇, Ser₁₉₉-Asp₂₀₆ and Asp₂₀₈-Phe₄₀₅; 10 three cacodylate-modified cysteines: Cys₃₃₄, Cys₃₈₀ and Cys₃₉₂; and 73 solvent molecules modeled as water (2003 atoms).

*
$$R_{\text{sym}} = 100 \times \Sigma_{\text{hkl}} \Sigma_{\text{i}} \mid I_{\text{i}} - I \mid / \Sigma_{\text{hkl}} \Sigma_{\text{i}} I_{\text{i}}$$

† $R_{\text{der}} = 100 \times \Sigma_{\text{hkl}} \mid F_{\text{PH}} - F_{\text{H}} \mid / \Sigma_{\text{hkl}} \mid F_{\text{P}} \mid$

The occupancy for the two bromine sites is set to 35 electrons. The occupancies of the 15 iodine sites are relative to this value.

§Phasing power = $\langle FH \rangle$, $/ \langle \epsilon \rangle$, where $\langle FH \rangle$ is the mean calculated heavy atom structure factor amplitude and $\langle \epsilon \rangle$ is the mean estimated lack of closure.

 $4Rcullis = \langle \in \rangle / \langle iso \rangle$, where $\langle \in \rangle$ is the mean estimated lack of closure and $\langle iso \rangle$ is the isomorphous difference.

20 ¶Rcryst = 100 x Σ_{hkl} |F_o-Fc| / Σ_{hkl} |F_o| where F_o and F_c are the observed and calculated structure factor amplitudes (for data F/ σ > 2). The Rfree was calculated using 3% of the data, chosen randomly, and omitted from the refinement.

§ Correlation coefficient =
$$\Sigma_{hkl}$$
 ($|F_o| - |F_o|$) x ($|F_c| - |F_c|$)/ Σ_{hkl} ($|F_o| - |F_o|$)²x Σ_{hkl} ($|F_c| - |F_c|$)²

25

Example 10. Phasing of the rTR- α LBD and hTR- β LBD complex with Triac

Due to the possible non-isomorphism of the rTRα LBD complex with Triac, a molecular replacement solution is determined using AMORE (Navaza, J., Acta 30 Crystallographica Section A-Fundamentals of Crystallography (1994) 50:157-63 from a starting model consisting of rTRI LBD complex with T₃, but with the ligand, all water molecules, and the following residues omitted: Asn 179, Arg228, Arg262, Arg266, and Ser 277. Strong peaks are obtained in both the rotation and translation

searches, with no significant (> 0.5 times the top peak) false solutions observed (Table 6). Strong positive density present in both the anomalous and conventional difference Fourier maps confirm the solution. Maps are calculated using sigma-A weighted coefficients output by REFMAC (Murshudov, et al. "Application of 5 Maximum Likelihood Refinements," in Refinement of Protein Structures, Proceedings of Daresbury Study Weekend (1996)) after 15 cycles of maximum likelihood refinement. Triac, the omitted residues, and water molecules 503, 504, 534 (following the numbering convention for the TR complex with T3) are built into the resulting difference density using O (Jones et. al.); the conformations of these residues are further confirmed in a simulated-annealing omit map (Brunger et. al.). The complete model is then refined using positional least-squares, simulated annealing, and restrained, grouped B factor refinement in XPLOR to an Reryst of 23.6% and an Rfree of 24.1%

Phasing of a related LBD using the structure of the rTR- α LBD is conducted 15 as follows. A molecular replacement solution for the hTR-β LBD complex with Triac is determined using AMORE from a starting model consisting of the rTR-a LBD complexed with T3, but with the ligand and all water molecules omitted. Strong peaks are obtained in both the rotation and translation searches, with no significant (>0.5 times the top peak) false solutions (Table 7). Strong positive density present in 20 both the anomalous and conventional difference Fourier maps confirm the solution. Initial maps are calulated using sigma-A weighted coefficients output by REFMAC after 9 cycles of maximum likelihood refinement. The real-space fit for each residues was calculated using OOPS (Kleywegt, GJ and Jones, TA, OOPS-a-daisy, ESF/CCP4 Newsletter 30, June 1994, pp. 20-24) and the residues with a real-space fit less than 2 25 standard deviations below the mean removed: Ala253-Lys263; Glu245-Leu250. To reduce bias, the following residues were modeled as alanine: Arg282, Arg316, Arg 320, Asn 331: Cycles of rebuilding and positional least-squares, simulated annealing, and restrained, grouped B factor refinement with XPLOR produce a model with an R_{cryst} of 25.3 and an R_{free} of 28.9%. The final model consists of hTR-β LBD residues 30 Glu202-Gln252, Val264-Glu460; three cacodylate-modified cysteines with the cacodylate moeity modeled as free arsenic: Cys294, Cys298, Cys388, and Cys434; and 35 solvent molecules modeled as water.

EXAMPLE 11. CONNECTING QSAR WITH STRUCTURE IN THE THYROID HORMONE RECEPTOR

The conclusions of classic thyroid hormone receptor quantitative structureactivity relationships may be summarized as follows:

- 5 1) the R₄'-hydroxyl group functions as a hydrogen bond donor;
 - 2) the amino-propionic acid interacts electrostatically through the carboxylate anion with a positively charged residue from the receptor;
 - 3) the preferences of R_3/R_5 substituent are I>Br>Me>>H;
 - 4) the preferences of the R₃'-substituent are Ipr>I>Br>Me>>H.
- 10 The structure of the thyroid hormone receptor ligand binding domain complexed with the agonists T3, IpBr₂, Dimit, Triac, and GC1 as provided herein, permits:
 - the identification of receptor determinants of binding at the level of the hydrogen bond;
 - the association of these determinants with the predictions of classic thyroid hormone receptor QSAR; and
 - 3) prediction as to which determinants of binding are rigid, and which are flexible, for both the ligand and the receptor.

This classification for the agonists of the type (R_1 =amino-propionic, acetic acid; R_3,R_5 =I,Br,Me; R_3 '=Ipr,I) is given below (for the representative ligand T_3);

20

15

F = Fiducial (always satisfied)

A = Adjustable

30

Based upon the methods and data described herein, the following is an embodiment of the computational methods of the invention, which permit design of nuclear receptor ligands based upon interactions between the structure of the amino acid residues of the receptor LBD and the four different ligands described herein. The

small molecule structures for the ligands can be obtained from Cambridge Structural Database (CSD), and three dimensional models can be constructed using the methods described throughout the specification. The following are factors to consider in designing synthetic ligands:

- 1) Histidine 381 acts as a hydrogen bond acceptor for the R₄' hydroxyl, with the optimal tautomer maintained by water molecules. See FIG. 23 and FIG 24. Histidine is the only hydrophilic residue in this hydrophobic pocket that surrounds the R₄' substituent. Histidine can be either a hydrogen bond acceptor or donor, depending on its tautomeric state. It is preferably a hydrogen bond donor, but can tolerate being a hydrogen bond acceptor, as for example, when there is a methoxy at the R₄' position of the ligand;
- Arginines 228, 262, and 266 interact directly and through water-mediated hydrogen bonds with the R₁-substituent, with the electrostatic interaction provided by Arginine 266 (as in the Triac complex). This polar pocket is illustrated by FIG. 23 -15 FIG. 25. FIG. 23 depicts T₃ in the TRI ligand binding cavity, where T3's aminopropionic R₁- substituent interacts with Arg 228, HOH502, H9H503 and HOH504 via hydrogen bonds. FIG. 24 depicts Triac in the ligand binding cavity, with its -COOH R₁ substituent in the polar pocket. In FIG. 24, Arg 228 no longer shares a hydrogen bond with the ligand, but the -COOH R₁ substituent forms hydrogen bonds with Arg 20 266. FIG. 25 superimposes T₃ and Triac in the ligand binding cavity and shows several positionally unchanged amino acids and water molecules, and selected changed interacting amino acids and water molecules. The three figures illustrate parts of the polar pocket that can change and those parts that do not move upon binding of different ligands. For example, the Arg 262 at the top of the polar pocket 25 does not move, even when the R₁ substituent has changed from a -COOH to an aminopropionic acid group. However, the other two Arginines, Arg 228 and Arg 266, demonstrate flexibility in the polar pocket to respond to the change in the size or chemical naure of the R₁ substituent.
- 3) Inner and outer pockets for the R₃/R₅ substituents are formed by 30 Ser260, Ala263, Ile299; and Phe 218, Ile221, Ile222, respectively. See FIGS. 21 and 22. The inner pocket is filled by either the R₃ or the R₅ substituent, regardless of the size of the substituent, and may act as a binding determinant by positioning the ligand in the receptor. Optimally, the inner pocket amino acids interact with an R₃ or R₅

substituent that is no larger than an iodo group. If the inner pocket is filled by the R₃ substituent, then the outer pocket interacts with the R₅ substituent and vice versa. The outer pocket can adjust to the size of its substituent through main chain motion centered at the break in helix 3 (Lys220-Ile221), suggesting that the bending of H3, and motion of the N-terminal portion of H3, may represent a conformational change induced on ligand binding. The outer pocket has greater flexibility than does the inner pocket in terms of accommodating a larger substituent group.

4) A pocket for the R₃'-substituent is formed by Phe 215, Gly290, Met388. The pocket is incompletely filled by the R₃'-iodo substituent, and 10 accommodates the slightly larger 3'-isopropyl substituent by movement of the flexible Met388 side chain and the H7/H8 loop. This pocket can accommodate R₃' substituents that are even larger than isopropyl, for example, a phenyl group.

The above information will facilitate the design of high affinity agonists and antagonists by improving automated QSAR methodologies and informing manual modeling of pharmaceutical lead compounds. For example, the inclusion of discrete water molecules provides a complete description of hydrogen bonding in the polar pocket for use with pharmacophore development: also, the identification of mobile and immobile residues within the receptor suggests physically reasonable constraints for use in molecular mechanics/dynamics calculations.

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EXAMPLE 12. DESIGN OF AN INCREASED AFFINITY LIGAND

Direct interaction between the receptor and the ligand is limited in the polar pocket, which interacts with the R₁ substituent. While the lack of complementarity may contain implications for biological regulation, it also provides an opportunity for increasing affinity by optimizing the interaction between the amino acids of the polar pocket and the R₁ substituent of a synthetic ligand. The structure of the receptor-ligand interactions described herein enables design of an increased affinity synthetic ligand having two complementary modifications:

1) Remove the positively charged amine. The strongly positive 30 electrostatic potential predicted for the polar pocket suggests that the positively charged amine of the aminopropionic acid R₁ substituent may be detrimental to binding. Suitable groups for substitution are suggested by the nature of nearby hydrogen bond partners: for example, Thr 275 O or Ser 277 N. See e.g. Tables in Appendix 2. For example, any any negatively charged substituent would be

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compatible for interacting with the amino acids of the polar pocket, including carboxylates, carbonyl, phosphonates, and sulfates, comprising 0 to 4 carbons. Another example of an R₁ substitution is an oxamic acid that replaces the amine of the naturally occurring ligand with one or more carbonyl groups.

Incorporate hydrogen bond acceptor and donor groups into the R₁-5 2) substituent to provide broader interactions with the polar pocket scaffold. Such hydrogen bond acceptor and donor groups incorporated into the R1-substituent will allow interactions that would otherwise occur with water molecules in the polar pocket. Specific waters include HOH 504 (hydrogen bonds with Ala 225 O and Arg 10 262 NH); and HOH 503 hydrogen bonds with Asn 179 OD1, Ala 180 N), both of which are present in all four complexes (TR LBD complexed with T3, TR LBD complexed with IpBr2, TR LBD complexed with Dimit and TR LBD complexed with Triac). Analysis of the hydrogen bonding network in the polar pocket suggests replacement of HOH 504 with a hydrogen bond acceptor, and HOH 503 with an 15 hydrogen bond donor (although the chemical nature of asparagine probably permits flexibility at this site). Thus, incorporating a hydrogen bond acceptor in an R1 substituent that could take the place of the HOH504 or incorporating a hydrogen bond acceptor in an R1 substituent that could positionally replace the HOH503, or a combination thereof, are methods of designing novel synthetic TR ligands.

20 These two design approaches can be used separately or in combination to design synthetic ligands, including those in Table 5 (below).

A corollary to this approach is to design specific interactions to the residues Arg262 and Asn 179. The goal is to build in interactions to these residues by designing ligands that have R₁ substituents that form hydrogen bonds with water 25 molecules or charged residues in the polar pocket.

High-affinity ligands also may be designed and selected using small molecules that bind to proximal subsites of the target nuclear hormone receptor that are identified in a structure-based screen and then linked together in their experimentally determined bound orientiations. Such a method has been described in design of high-30 affinity ligands for the FK506 binding protein (FKBP), stromelysin, gelatinase A, and human papillomavirus E2 (Hajduk et al., Science 278:497-499 (1997)), which reference and its references are incorporated herein by reference. The preferred small molecules for screening are compounds of Formula I or derivatives thereof. For

example, a compound of Formula I (φ-X-φ) or a derivative thereof (φ-X or X-φ) is screened for binding a target nuclear hormone receptor LBD. Proximal subsites of the nuclear hormone receptor include the hydrophobic and polar pockets of the LBD, and substites extended therefrom. As an example, Fourier transformation or nuclear magnetic resonance (NMR) -based structure screens can be used. When a NMR-based screen is used, binding can be detected from the amide chemical shift changes observed in two-dimensional heteronuclear single quantum correlation (HSQC) spectra aquired in the presence and absence of added compound. Once two ligands are identified that bind to the receptor, the crystal or solution structure of the ternary complex is determined. From the structural information, a compound is synthesized which links the two ligands, where the linker is selected based on structural information. The new compound is then screened for binding affinity, for example, using a binding assay as described herein. Only a few linked ligands need to synthesized and screened when using this approach.

15 Compounds of the invention also may be interatively designed from structural information of the compounds described above using other structure-based design/modeling techniques (Jackson, R.C., Contributions of protein structure-based drug design to cancer chemotherapy. Semninars in Oncology, 1997, 24(2)L164-172; and Jones, T.R., et al., J. Med. Chem., 1996 39(4):904-917).

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Table 5: Synthetic TR Ligands

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R1	R2	R3	R5	R6	x	R'2	R'3	R'4	R'5	R'6
СО2Н	Н	Me	Me	Н	0	Н	Me	ОН	Me	Н
СН2СО2Н		1	1		s		Et	SH	Et	
CH2CH2CO2H		Br	Br				nPr	NH2	nPr	
CH2CH(NH2)CO2H		Cl	CI				iPr		iPr	
ОСН2СО2Н		Et	Et				Ph		nBu	
ОСН2СН2СО2Н		ОН-	ОН				I		nPen	
NHCH2CO2H		NH2	NH2				Br		nHex	
NHCH2CH2CO2H		SH	SH				Cl		Ph	
СН2СОСОСО2Н									hetero	
•			÷						cycle	
NHCOCOCO2H									aryl	
СОСО2Н										
CF2CO2H										
COCH2CO2H										

Any combination of the above substituents in the biphenyl ether scaffold structure shown above may result in a potentially pharmacologically useful ligand for the 10 thyroid hormone receptor. These novel ligands may be antagonists of the thyroid receptor.

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TABLE 6: TR-α LBD-122/410

	IAD	EE U. IK-a ED	D-122/410	
	Dimit '	Т3	lpBr ₂	Triac
Data collection				
Cell dimensions	-			
a (Å)	117.16	117.19	117.18	118.19
b (Å)	80.52	80.20	80.12	81.37
c (Å)	63.21	63.23	63.13	63.73
β (°)	120.58	120.60	120.69	121.00
Resolution (Å)	2.2	2.0	2.1	2.45
Obs. Reflections, (no.)	57031	64424	66877	83573
Unique Reflections, (no.)	22327	21023	23966	18453
Completeness, (%)	87.0	82.4	93.7	96.0
*R _{svm} (%)	3.9	3.5	4.5	7.5
Phasing (15.0 - 2.5Å)				
†R _{der} (%)	• - ·	19.6	11.6	
No. of sites	-	3	2	
‡Occupancy	-	44.6 (19.8)	35.0	
(Anomalous)	-	50.2 (23.7)	35.0	
•		39.2 (22.3)		
§F _H /E				
centric (acentric)		,		
15.0-5.0 Å	-	3.67 (4.61)	2.25 (3.09)	.*
5.0-3.0 Å	-	2.23 (2.75)	1.25 (1.85)	
3.0-2.5 Å	•	1.64 (1.99)	1.15 (1.57)	
¶R _{Cullis} (%)				
15.0-5.0 Å	-	33	44	
5.0-3.0 Å	-	45	63	
3.0-2.5 Å	•	60	65	
Mean figure of merit	0.62	-	•	
MR Phasing (10-3.5Å)				
Rotation Search:	-			$\Theta_1 = 309.37$
Euler Angles (°)				$\Theta_2 = 48.96$
•		•		$\Theta_3 = 127.28$
§ correlation coefficient				34.3
Translation Search: Fractional coordinates		·		x = 0.1571
				y = 0.000
				z = 0.3421
§ correlation Coefficient				z = 0.3421 65.8

Refinement Resolution (Å)	15.0-2.2	5.0 - 2.0	15.0 - 2.2	25-2,5
¶R _{cryst (%)}	20.5	22.1	21.4	23.6
R _{free (%)}	22.7	24.0	22.4	24.1

TABLE 7: TR-β LBD-202/461

	Triac	Т3	GCI
Data collection			
Space Group	-	P3121	
Cell dimensions			
a (Å)	68.9	68.45	68.73
c (Å)	131.5	130.56	130.09
Resolution (Å)	2.4	3.1	2.8
Obs. Reflections. (no.)	80196	55103	54104
Unique Reflections. (no.)	14277	6847	8987
Coverage (%)	97.0	95.7	97.1
*R _{sym} (%)	5.1	4.6	5.5
MR Phasing (15.0 - 3.5Å)			
Rotation Search	$\Theta_1 = 39.13$		
Euler Angles (°)	Θ ₂ =68:00		
	Θ₃=323.6		
§ correlation coefficient	21.6		
(Highest false peak)	(10.8)		
Translation Search	x=0.748		
Fractional Coordinates	y=0.158		
	z=0.167		
§ correlation coefficient	57.5		
(Highest false peak)	(38.7)		
	0.612		
*R factor	40.7	40.8	
Refinement			
Resolution (Å)	30-2.4		30-2.9
¶R _{cryst (%)}	- _{25.3}		27.3
R _{free (%)}	28.9		33.4

All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference. The nuclear receptor ligands, particularly the TR ligands, of these

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references are herein incorporated by reference and can be optionally excluded from the claimed compounds with a proviso.

Headings and subheadings are presented only for the convenience of the reader and should not be used to construe the meaning of terms used within such 5 headings and subheadings.

The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

A method of modulating the activity of a thyroid hormone receptor
 (TR) which comprises administering to a mammal in need thereof a compound of the
 formula:

wherein said compound fits spatially and preferentially into a TR ligand binding domain (TR LBD) and comprises the following substituents:

- (i) an R₁-substituent comprising an anionic group that interacts with a side 15 chain nitrogen atom of an arginine corresponding to a residue selected from the group consisting of Arg228, Arg262, and Arg266 of human TR-α, and Arg282, Arg316 and Arg320 of human TR-β, and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;
- (ii) an R₂-substituent comprising a hydrophobic or hydrophilic group that
 20 fits spacially into the TR LBD;
- (iii) an R₃-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue selected from the group consisting of Ser260, Ala263 and Ile299 of human TR-α, and Ser314, Ala317 and Ile352 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

(iv) an R₅-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected from the group consisiting of Phe218, Ile221 and Ile222 of human TR-I, and Phe272, Ile275 and Ile276 of human TR-β, and wherein the hydrophobic or 5 hydrophilic group is 1.7-4.0Å from the side chain atom;

- (v) an R₆-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a leucine corresponding to a residue selected from the group consisting of Leu276 and Leu292 of human TR-α, and Leu 330 and Leu346 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;
 - (vii) an R_2 '-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- 15 (viii) an R₃'-substituent comprising a hydrophobic group that interacts with a side chain atom of a phenylalamine, glycine or methionine corresponding to a residue selected from the group consisting of Phe215, Gly290, and Met388 of human TR-α, and Phe269, Gly344, Met442 of human TR-β, and wherein the hydrophobic group is 1.7-4.0Å from the side chain atom;
- 20 (ix) an R₄'-substituent comprising an hydrogen bond donor or acceptor group that interacts with a side chain carbon or nitrogen atom of a histadine corresponding to residue His381 of human TR-α, and His435 of human TR-β, and wherein the hydrogen bond donor or acceptor group is 1.7-4.0Å from the side chain atom;

(x) an R₅'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;

- (xi) and R₆'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- wherein said compound is other than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I, and wherein the activity of said TR is modulated.
 - 2. The method according to claim 1,
- 10 wherein R₁ is
 - -O-CH2CO2H, -NHCH2CO2H,
 - -CO₂H, -CH₂CO₂H, -CH₂CH₂CO₂H, -CH₂CH₂CO₂H,
 - -CH₂CH(NH₂)CO₂H,

-CH₂CH[NHCOCHφ₂]CO₂H,

- -CH₂CH[NHCO(CH₂)₁₅CH₃
-]CO₂H,
- -CH₂CH[NH-FMOC]CO₂H,
- -CH₂CH[NH-tBOC]CO₂H, or a carboxylate connected to the ring with a 0 to 3 carbon linker,
 - $-PO_{3}H_{2}, \qquad -CH_{2}PO_{3}H_{2}, \qquad -CH_{2}CH_{2}PO_{3}H_{2}, \qquad -CH_{2}CHNH_{2}PO_{3}H_{2},$
 - $-CH_2CH[NHCOCH_{\phi_2}]PO_3H_2, \\ -CH_2CH[NHCO(CH_2)_{15}CH_3]PO_3H_2, \\$
- -CH₂CH[NH-FMOC]PO₃H₂, -CH₂ CH[NH-tBOC]PO₃H₂, or a phosphate or phosphonate connected to the ring with a 0 to 3 carbon linker,

-CH₂CH[NH-FMOC]SO₃H, -CH₂ CH[NH-tBOC]SO₃H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon linker,

or acts as the functional equivalent of CH₂CH(NH₂)CO₂H of T3 in the molecular recognition domain when bound to a TR, wherein said R₁ can be optionally substituted with an amine,

wherein R2 is

H, halogen, CF₃, OH, NH₂, SH, CH₃, -Et,

or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein R₃ is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et,

or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

wherein R5 is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR, and R₃ can be identical to R₅,

wherein R₆ is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR, and R₂ can be identical to R₆,

5 wherein R₂' is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein R₃' is any hydrophobic group, including

halogen, -CF₃, -SH, alkyl, aryl, 5- or 6-membered heterocyclie, cyano, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

wherein R₄' is

-H, halogen, -CF₃, -OH, -NH₂, NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, -SH, -CH₃, -Et, or akyl, aryl or 5- or 6-membered heterocyclic aromatic attached through urea or carbamate linkages to O or N or S at the R₄' position, or acts as the functional equivalent of OH in the molecular recognition domain when bound to a TR,

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wherein R5' is

-H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally

connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups,

wherein R₆' is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein X is

O, S, SO₂, NH, NR₇, CH₂, CHR₇, CR₇R₇, wherein R₇ is alkyl, aryl or 5- or 6-membered heterocyclic aromatic,

15

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and wherein said TR LBD ligand has an apparent Kd for binding TR LBD of 1 TM or less.

- 3. The method of claim 2, wherein
- R_1 is carboxylate, phosphonate, phosphate or sulfite and is connected to the ring with a 0 to 3 carbon linker,

R₂ is H,

 R_3 is -I, -Br, or -CH₃,

 R_5 is -I, -Br, or -CH₃,

25 R₆ is H,

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R₂' is H,

R₃' is -I, -Br, -CH₃, -iPr, -phenyl, benzyl, or 5- or 6-membered ring heterocycles.

R₄' is -OH, -NH₂, and -SH,

R₅' is -H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 10 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups, and

15 R₆' is H.

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- The method of claim 1, wherein said compound fits spatially and 4. preferentially into TR LBD isoform α (TR- α).
- 20 5. The method of claim 4, wherein said compound comprises an anionic group that interacts with the side chain oxygen or carbon of a serine residue corresponding to Ser277 of human TR-α, and wherein the anionic group is 1.7-4.0Å from the side chain atom.

6. The method of claim 1, wherein said compound fits spatially and preferentially into TR LBD isoform β (TR- β).

- The method of claim 6, wherein said compound comprises an anionic
 group that interacts with the side chain nitrogen of an arginine corresponding to
 Asn331 of human TR-β, and the anionic group is 1.7-4.0Å from the side chain atom.
- 8. A method for identifying a compound capable of selectively modulating the activity of a thyroid hormone receptor (TR) isoform, said method 10 comprising:

modeling test compounds that fit spacially and preferentially into a TR ligand binding domain (TR LBD) isoform of interest using an atomic structural model of a TR LBD isoform bound to a test compound,

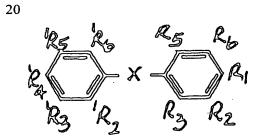
screening said test compounds in a biological assay for TR isoform

15 activity characterized by binding of a test compound to a TR LBD isoform, and

identifying a test compound that selectively modulates the activity of a

TR isoform.

9. The method of claim 8, wherein said compound is of the formula:



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which comprises the following substituents:

- (i) an R₁-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue selected from the group consisting of Arg228, Arg262, and Arg266 of human TR-α, and Arg282, Arg316 and 5 Arg320 of human TR-β, and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;
 - (ii) an R₂-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- (iii) an R₃-substituent comprising a hydrophobic or hydrophilic group that 10 interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue selected from the group consisting of Ser260, Ala263 and Ile299 of human TR-α, and Ser314, Ala317 and Ile352 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;
- (iv) an R₅-substituent comprising a hydrophobic or hydrophilic group that
 15 interacts with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected from the group consisiting of Phe218, Ile221 and Ile222 of human TR-α, and Phe272, Ile275 and Ile276 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;
- (v) an R₆-substituent comprising a hydrophobic or hydrophilic group that
 20 fits spacially into the TR LBD;
- (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a leucine corresponding to a residue selected from the group consisting of Leu276 and Leu292 of human TR-α, and Leu 330 and Leu346 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from 25 the side chain atom;

(vii) an R₂'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;

- (viii) an R₃'-substituent comprising a hydrophobic group that interacts with a side chain atom of a phenylalamine, glycine or methionine corresponding to a residue
 5 selected from the group consisting of Phe215, Gly290, and Met388 of human TR-α, and Phe269, Gly344, Met442 of human TR-β, and wherein the hydrophobic group is
 1.7-4.0Å from the side chain atom;
- (ix) an R₄'-substituent comprising an hydrogen bond donor or acceptor group that interacts with a side chain carbon or nitrogen atom of a histadine 10 corresponding to residue His381 of human TR-α, and His435 of human TR-β, and wherein the hydrogen bond donor or acceptor group is 1.7-4.0Å from the side chain atom;
 - (x) an R_5 '-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD; and
- 15 (xi) and R₆'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD.
 - 10. The method according to claim 9, wherein R_1 is
- 20 -O-CH₂CO₂H, -NHCH₂CO₂H,
 - $-\text{CO}_2\text{H}, -\text{CH}_2\text{CO}_2\text{H}, -\text{CH}_2\text{CH}_2\text{CO}_2\text{H}, -\text{CH}_2\text{CH}_2\text{CO}_2\text{H}, \\$
 - -CH₂CH(NH₂)CO₂H,

- $CH_2CH[NHCOCH\phi_2]CO_2H$,

- -CH₂CH[NHCO(CH₂)₁₅CH₃
-]CO₂H,
- -CH2CH[NH-FMOC]CO2H,
- -CH₂CH[NH-tBOC]CO₂H, or a carboxylate connected to the ring with a 0 to 3
- 25 carbon linker,

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-PO₃H₂, -CH₂PO₃H₂, -CH₂CH₂PO₃H₂, -CH₂CHNH₂PO₃H₂,
-CH₂CH[NHCOCHφ₂]PO₃H₂, -CH₂CH[NHCO(CH₂)₁₅CH₃]PO₃H₂,
-CH₂CH[NH-FMOC]PO₃H₂, -CH₂ CH[NH-tBOC]PO₃H₂, or a phosphate or phosphonate connected to the ring with a 0 to 3 carbon linker,

-SO₃H, -CH₂SO₃H, -CH₂CH₂SO₃H, -CH₂CHNH₂SO₃H,
-CH₂CH[NHCOCHφ₂]SO₃H, -CH₂CH[NHCO(CH₂)₁₅CH₃]SO₃H,
-CH₂CH[NH-FMOC]SO₃H, -CH₂ CH[NH-tBOC]SO₃H, or a sulfate or sulfite

10 connected to the ring with a 0 to 3 carbon linker,

or acts as the functional equivalent of CH₂CH(NH₂)CO₂H of T3 in the molecular recognition domain when bound to a TR, wherein said R₁ can be optionally substituted with an amine,

15

wherein R₂ is

H, halogen, CF₃, OH, NH₂, SH, CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

20

wherein R₃ is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

25

wherein R₅ is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR, and R_3 can be identical to R_5 ,

5

wherein R₆ is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR, and R₂ can be identical to R₆,

10

wherein R₂' is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

15 wherein R₃' is any hydrophobic group, including

halogen, -CF₃, -SH, alkyl, aryl, 5- or 6-membered heterocyclie, cyano, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

20 wherein R₄' is

25

-H, halogen, -CF₃, -OH, -NH₂, NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, -SH, -CH₃, -Et, or akyl, aryl or 5- or 6-membered heterocyclic aromatic attached through urea or carbamate linkages to O or N or S at the R₄' position, or acts as the functional equivalent of OH in the molecular recognition domain when bound to a TR,

wherein R5' is

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-H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups,

wherein R₆' is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein X is

O, S, SO₂, NH, NR₇, CH₂, CHR₇, CR₇R₇, wherein R₇ is alkyl, aryl or 5- or 6-membered heterocyclic aromatic,

and wherein said TR LBD ligand has an apparent Kd for binding TR LBD of 1 TM or less.

25 11. The method of claim 10, wherein

R₁ is carboxylate, phosphonate, phosphate or sulfite and is connected to the ring with a 0 to 3 carbon linker,

R₂ is H,

R₃ is -I, -Br, or -CH₃,

 R_5 is -I, -Br, or -CH₃,

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R₆ is H,

R₂' is H,

 R_3 ' is -I, -Br, -CH₃, -iPr, -phenyl, benzyl, or 5- or 6-membered ring heterocycles,

10 R_4 ' is -OH, -NH₂, and -SH,

R₅' is -H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups, and

. R₆' is H.

12. The method of claim 8, wherein said compound fits spatially and preferentially into TR LBD isoform α (TR- α).

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13. The method of claim 12, wherein said compound comprises an anionic group that interacts with the side chain oxygen or carbon of a serine residue corresponding to Ser277 of human TR- α , and wherein the anionic group is 1.7-4.0Å from the side chain atom.

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- 14. The method of claim 8, wherein said compound fits spatially and preferentially into TR LBD isoform β (TR- β).
- 15. The method of claim 14, wherein said compound comprises an anionic 10 group that interacts with the side chain nitrogen of an arginine corresponding to Asn331 of human TR-β, and the anionic group is 1.7-4.0Å from the side chain atom.
 - 16. The method of claim 8, wherein said compound binds to a TR LBD isoform with greater affinity than thyronine or triidothyronine.

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17. A method for identifying a thyroid hormone receptor (TR) agonist or antagonist ligand, said method comprising the steps of:

providing the atomic coordinates of a TR ligand binding domain (TR LBD) to a computerized modeling system;

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modeling ligands which fit spacially into the TR LBD; and

identifying in a biological assay for TR activity a ligand which increases or descreases the activity of said TR, whereby a TR agonist or antagonist is identified.

18. A peptide, peptidomimetic or synthetic molecule identified by the method of any one of claims 8 or 17, with the proviso that said molecule is other than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I.

5 19. A method of identifying a compound that selectively modulates the activity of a thyroid hormone receptor (TR) compared to other nuclear hormone receptors, said method comprising:

modeling compounds which fit spacially into a TR ligand binding domain (TR LBD) using an atomic structural model of a TR LBD,

selecting a compound comprising conformationally constrained structural features that interact with conformationally constrained residues of a TR LBD,

identifying in a biological assay for TR activity a compound that selectively binds to a TR LBD compared to other nuclear receptors, whereby a 15 compound that selectively modulates a TR is identified.

- 20. The method of claim 19, wherein said conformationally constrained residues of a TR LBD correspond to residues Met259, Leu276, Leu292, His381, Gly290, Ile221, and Phe401 of human TR-α, and residues Met313, Leu330, Leu346, 20 His435, Gly344, Ile275 and Phe455 of human TR-β.
 - 21. The method of claim 19, wherein said compounds are of the formula:

which comprises the following substituents:

- (i) an R₁-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue selected from the group 10 consisting of Arg228, Arg262, and Arg266 of human TR-α, and Arg282, Arg316 and Arg320 of human TR-β, and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;
 - (ii) an R₂-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- 15 (iii) an R₃-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue selected from the group consisting of Ser260, Ala263 and Ile299 of human TR-α, and Ser314, Ala317 and Ile352 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;
- 20 (iv) an R₅-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected from the group consisting of Phe218, Ile221 and Ile222 of human TR-α, and Phe272, Ile275 and Ile276 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

(v) an R₆-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;

- (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a leucine corresponding to a residue selected from
 5 the group consisting of Leu276 and Leu292 of human TR-α, and Leu 330 and Leu346 of human TR-β, and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;
 - (vii) an R₂'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;
- 10 (viii) an R₃'-substituent comprising a hydrophobic group that interacts with a side chain atom of a phenylalanine, glycine or methionine corresponding to a residue selected from the group consisting of Phe215, Gly290, and Met388 of human TR-α, and Phe269, Gly344, Met442 of human TR-β, and wherein the hydrophobic group is 1.7-4.0Å from the side chain atom;
- 15 (ix) an R₄'-substituent comprising an hydrogen bond donor or acceptor group that interacts with a side chain carbon or nitrogen atom of a histidine corresponding to residue His381 of human TR-α, and His435 of human TR-β, and wherein the hydrogen bond donor or acceptor group is 1.7-4.0Å from the side chain atom;
- 20 (x) an R₅'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD; and
 - (xi) and R_6 '-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD.
- 25 22. The method of claim 19, wherein said compound comprises:

 (i) a cyclic carbon atom that interacts with a carbon and oxygen atom of a methionine residue corresponding to Met259 of human TR-α, and Met313 of human TR-β, wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon and oxygen atom of the methionine;

- 5 (ii) a cyclic carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu276 of human TR-α, and Leu330 of human TR-β, wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine;
- (iii) a cyclic carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu292 of human TR-α, and Leu346 of human TR-β,
 10 wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine;
 - (iv) a R₃-substituent comprising an atom that interacts with a carbon atom of an isoleucine residue corresponding to Ile221 of human TR-α, and Ile275 of human TR-β, wherein the R₃-substituent atom is about 3.0 to 4.0Å from the carbon atom of the isoleucine;
- 15 (v) a R₃'-substituent comprising an atom that interacts with an oxygen atom of a glycine residue corresponding to Gly290 of human TR-α, and Gly344 of human TR-β, wherein the R3'-substituent atom is about 3.0 to 4.0Å from the carbon atom of the glycine; and
- (vi) a R₄'-substituent comprising an atom selected from the group 20 consisting of oxygen and carbon that interacts with (a) a carbon and nitrogen atom of a histidine residue corresponding to His381 of human TR-α, and His435 of human TR-β, wherein the R4'-substituent atom is about 2.0 to 4.0Å from the carbon atom of the histidine; and (b) a carbon atom of a phenylalanine residue corresponding to Phe401 of human TR-α, and human Phe455 of TR-β, wherein said atom is about 3.0 to 4.0Å from the carbon atom of the phenylalanine.

23. The method according to claim 21,

wherein R1 is

-O-CH₂CO₂H, -NHCH₂CO₂H,

5 -CO₂H, -CH₂CO₂H, -CH₂CH₂CO₂H, -CH₂CH₂CO₂H,

-CH₂CH(NH₂)CO₂H, -CH₂CH[NHCOCHφ₂]CO₂H,

-CH₂CH[NHCO(CH₂)₁₅CH₃]CO₂H, -CH₂CH[NH-FMOC]CO₂H,

-CH₂CH[NH-tBOC]CO₂H, or a carboxylate connected to the ring with a 0 to 3

carbon linker,

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 $-PO_3H_2$, $-CH_2PO_3H_2$, $-CH_2CH_2PO_3H_2$, $-CH_2CHNH_2PO_3H_2$,

 $-CH_2CH[NHCOCH\varphi_2]PO_3H_2, \\ -CH_2CH[NHCO(CH_2)_{15}CH_3]PO_3H_2, \\$

-CH₂CH[NH-FMOC]PO₃H₂, -CH₂ CH[NH-tBOC]PO₃H₂, or a phosphate or

phosphonate connected to the ring with a 0 to 3 carbon linker,

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 $-SO_3H, \qquad -CH_2SO_3H, \qquad -CH_2CH_2SO_3H, \qquad -CH_2CHNH_2SO_3H, \\$

 $-CH_2CH[NHCOCH\phi_2]SO_3H, \qquad -CH_2CH[NHCO(CH_2)_{15}CH_3]SO_3H, \\$

-CH2CH[NH-FMOC]SO3H, -CH2 CH[NH-tBOC]SO3H, or a sulfate or sulfite

connected to the ring with a 0 to 3 carbon linker,

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or acts as the functional equivalent of CH₂CH(NH₂)CO₂H of T3 in the molecular recognition domain when bound to a TR, wherein said R₁ can be

optionally substituted with an amine,

25 wherein R₂ is

H, halogen, CF₃, OH, NH₂, SH, CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

5 wherein R₃ is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

10 wherein R₅ is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR, and R_3 can be identical to R_5 ,

15 wherein R₆ is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR, and R₂ can be identical to R₆,

20 wherein R₂' is

-H, halogen, -CF₃, -OH, -NH₂, -N₃, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein R₃' is any hydrophobic group, including

halogen, -CF₃, -SH, alkyl, aryl, 5- or 6-membered heterocycle, cyano, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

5 wherein R₄' is

-H, halogen, -CF₃, -OH, -NH₂, NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, -SH, -CH₃, -Et, or akyl, aryl or 5- or 6-membered heterocyclic aromatic attached through urea or carbamate linkages to O or N or S at the R₄' position, or acts as the functional equivalent of OH in the molecular recognition domain when bound to a TR,

wherein R5' is

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-H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups,

wherein R₆' is

-H, halogen, -CF₃, -OH, -NH₂, -SH, -CH₃, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

wherein X is

O, S, SO₂, NH, NR₇, CH₂, CHR₇, CR₇R₇, wherein R₇ is alkyl, aryl or 5- or 6-membered heterocyclic aromatic,

and wherein said TR LBD ligand has an apparent Kd for binding TR LBD of 1 TM or less.

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24. The method of claim 23, wherein

R₁ is carboxylate, phosphonate, phosphate or sulfite and is connected to the ring with a 0 to 3 carbon linker,

R₂ is H,

15 R₃ is -I, -Br, or -CH₃,

 R_5 is -I, -Br, or -CH₃,

R₆ is H,

R₂' is H,

R₃' is -I, -Br, -CH₃, -iPr, -phenyl, benzyl, or 5- or 6-membered ring 20 heterocycles,

R₄' is -OH, -NH₂, and -SH,

R₅' is -H, -OH, -NH₂, -N(CH₃)₂ -SH -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is

optionally connected to the ring by a -CH₂-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH₂, -SH, -NH₃, -N(CH₃)₃, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said R₅' may be substituted with polar or charged groups, and

R₆' is H.

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- 25. The method of claim 19, wherein said compound fits spatially and 10 preferentially into TR LBD isoform α (TR- α).
- 26. The method of claim 25, wherein said compound comprises an anionic group that interacts with the side chain oxygen or carbon of a serine residue corresponding to Ser277 of human TR-α, and wherein the anionic group is 1.7-4.0Å 15 from the side chain atom.
 - 27. The method of claim 19, wherein said compound fits spatially and preferentially into TR LBD isoform β (TR- β).
- 28. The method of claim 27, wherein said compound comprises an anionic group that interacts with the side chain nitrogen of an arginine corresponding to Asn331 of human TR-β, and the anionic group is 1.7-4.0Å from the side chain atom.
- 29. The method of claim 19, wherein said compound binds to a TR LBD 25 isoform with greater affinity than thyronine or triiodothyronine.

30. The method of claim 1, wherein said compound comprises a cyclic carbon atom that interacts with a carbon and oxygen atom of a methionine residue corresponding to Met259 of human TR-I, and Met313 of human TR-β, wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon and oxygen atom of the methionine.

31. The method of claim 30, wherein said cyclic carbon is inner ring carbon C11.

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32. The method of claim 1, wherein said compound comprises a cyclic carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu276 of human TR-α, and Leu330 of human TR-β, wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine.

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- 33. The method of claim 32, wherein said cyclic carbon is selected from the group consisting of inner ring carbons C7 and C9.
- 34. The method of claim 1, wherein said compound comprises a cyclic 20 carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu292 of human TR-α, and Leu346 of human TR-β, wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine.
- 35. The method of claim 34, wherein said cyclic carbon is selected from 25 the group consisting of outer ring carbons C6 and C8.

36. The method of claim 1, wherein said R₃-substituent comprises an atom that interacts with a carbon atom of an isoleucine residue corresponding to Ile221 of human TR-α, and Ile275 of human TR-β, wherein the R₃-substituent atom is about
5 3.0 to 4.0Å from the carbon atom of the isoleucine.

- 37. The method of claim 1, wherein said R₃'-substituent comprises an atom that interacts with an oxygen atom of a glycine residue corresponding to Gly290 of human TR-α, and Gly344 of human TR-β, wherein the R₃'-substituent atom is 10 about 3.0 to 4.0Å from the carbon atom of the glycine.
- 38. The method of claim 1, wherein said R₄'-substituent comprises an atom selected from the group consisting of oxygen and carbon that interacts with a carbon and nitrogen atom of a histidine residue corresponding to His381 of human 15 TR-α, and His435 of human TR-β, wherein the R₄'-substituent atom is about 2.0 to 4.0Å from the carbon atom of the histidine.
- 39. The method of claim 1, wherein said R₄'-substituent comprises an oxygen atom that interacts with a carbon atom of a phenylalanine residue
 20 corresponding to Phe401 of human TR-α, and human Phe455 of TR-β, wherein said atom is about 3.0 to 4.0Å from the carbon atom of the phenylalanine.
- 40. A method for identifying a thyroid hormone receptor (TR) agonist or antagonist ligand that selectively modulates the activity of a TR compared to other 25 nuclear receptors, said method comprising the steps of:

providing the atomic coordinates of a TR ligand binding domain (TR LBD) to a computerized modeling system;

modeling ligands which fit spacially into the TR LBD and which interact with conformationally constrained residues of a TR LBD conserved among 5 TR isoforms; and

identifying in a biological assay for TR activity a ligand which selectively binds to said TR and increases or decreases the activity of said TR, whereby a TR agonist or antagonist that selectively modulates the activity of a TR is identified.

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- 41. A peptide, peptidomatic or synthetic molecule identified by the method of any one of claims 19 or 40, with the proviso that said molecule is other than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I.
- 15 42. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a thyroid hormone ligand binding pocket comprising structure coordinates of TR-α amino acids 20 corresponding to human TR-α amino acids Met259, Leu276, and Ile221, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

43. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a thyroid 5 hormone ligand binding pocket comprising structure coordinates of TR-α amino acids corresponding to human TR-α amino acids Leu292, His381, Gly290 and Phe401, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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44. The machine-readable storage medium according to any one of claims 42 or 43, wherein said binding pocket comprises structure coordinates of TR- α amino acids corresponding to human TR- α amino acids Met259, Leu276, Leu292, His381, Gly290, Ile221 and Phe401.

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- 45. The machine-readable storage medium according to claim 44, wherein said binding pocket comprises structure coordinates of TR-α amino acids corresponding to human TR-α amino acids Arg228, Arg262 and Arg266.
- 20 46. The machine-readable storage medium according to claim 44, wherein said binding pocket comprises structure coordinates of TR-α amino acids corresponding to human TR-α amino acids Ser260, Ala263 and Ile299.

47. The machine-readable storage medium according to claim 44, wherein said binding pocket comprises structure coordinates of TR- α amino acids corresponding to human TR- α amino acids Phe218, Ile221 and Ile222.

- 5 48. The machine-readable storage medium according to claim 44, wherein said binding pocket comprises structure coordinates of TR-α amino acids corresponding to human TR-α amino acids Phe215, Gly290 and Met388.
- 49. The machine-readable storage medium according to claim 44, wherein 10 said binding pocket comprises structure coordinates of a TR-α amino acid corresponding to human TR-α amino acid Ser277.
- 50. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a thyroid hormone ligand binding pocket comprising structure coordinates of TR-β amino acids corresponding to human TR-β amino acids Met313, Leu330, and Ile275, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 51. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical

three-dimensional representation of a molecule or molecular complex for a thyroid hormone ligand binding pocket comprising structure coordinates of TR-β amino acids corresponding to human TR-β amino acids Leu346, His435, Gly344, and Phe455, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 52. The machine-readable data storage medium according to any one of claims 50 or 51, wherein said binding pocket comprises structure coordinates of TR-β
 10 amino acids corresponding to human TR-β amino acids Met313, Leu330, Leu346, His435, Gly344, Ile275 and Phe455.
- 53. The machine-readable data storage medium according to claim 52,
 wherein said binding pocket comprises structure coordinates of TR-β amino acids
 15 corresponding to human TR-β amino acids Arg282, Arg316 and Arg320.
 - 54. The machine-readable data storage medium according to claim 52, wherein said binding pocket comprises structure coordinates of TR-β amino acids corresponding to human TR-β amino acids Ser314, Ala317 and Ile352.

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55. The machine-readable data storage medium according to claim 52, wherein said binding pocket comprises structure coordinates of TR-β amino acids corresponding to human TR-β amino acids Phe272, Ile275 and Ile276.

56. The machine-readable data storage medium according to claim 52, wherein said binding pocket further comprises structure coordinates of TR-β amino acids corresponding to human TR-β amino acids Phe269, Gly344 and Met442.

- 5 57. The machine-readable data storage medium according to claim 52, wherein said binding pocket comprises structure coordinates of a TR-β amino acid corresponding to human TR-β amino acid Asn331.
- 58. The machine-readable data storage medium according to claim 52, 10 wherein said molecule or molecular complex is defined by the set of structure coordinates selected from the group consisting coordinates depicted in Appendix 3, 4, 5 and 6, or a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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- 59. The machine-readable data storage medium according to claim 52, wherein said molecule or molecular complex is defined by the set of structure coordinates selected from the group consisting coordinates depicted in Appendix 7 and 8, or a homologue of said molecule or molecular complex, said homologue 20 having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 60. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined 25 with a second set of machine readable data, using a machine programmed with

instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 3, 4, 5, 6, 7 and 8; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

PCT/US98/25296

APPENDIX 1

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APPENDIX 2

Table 8

Dimit	Amino Acid	Amino Acid	Distance
Atom	in full length α	Atom	Å
C16	215-PHE	CD1	3.98
C16	215-PHE	CE1	3.86
C19	218-PHE	0	3.69
C16	218-PHE	СВ	3.89
C18	218-PHE	СВ	3.92
C19	218-PHE	СВ	4.13
C18	218-PHE	CD2	3.77
C16	219-THR	CG2	3.68
C19	221-ILE	CG1	4.11
C6	222-ILE	CD1	4.18
C8	222-ILE	CD1	3.72
C10	222-ILE	CD1	3.53
C12	222-ILE	CD1	3.85
01	222-ILE	CD1	4.13
C13	225-ALA	C8	3.64
04	225-ALA	C8	4.02
04	228-ARG	CZ	3.96
C17	228-ARG	NH2	3.36
O3	228-ARG	NH2	3.58
04	228-ARG	NH2	2.86
C10	256-MET	SD	3.70
C12	256-MET	SD	3.89
C10	256-MET	CE	3.88
C12	256-MET	CE	3.83
C11	259-MET	C	4.03
C11	259-MET	0	3.66
C15	259-MET	0	3.42
N1	259-MET	0	3.71
C1	259-MET	C8	4.20
C11	259-MET	C8	3.87
C13	259-MET	C8	4.09
C15	262-ARG	C8	4.03
C17	262-ARG	C8	3.58
O3	262-ARG	C8	3.62
04	262-ARG	C8	3.85
C17	262-ARG	CD	4.10
O4	262-ARG	CD	3.61
N1	263-ALA	N	3.71
C17	263-ALA	CA	3.69
N1	263-ALA	CB	3.46
O3	266-ARG	NH1	3.93

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Dimit	Amino Acid	Amino Acid	Distance
Atom	in full length α	Atom	Å
NI	275-THR	0	3.62
NI	276-LEU	CA	3.51
NI	276-LEU	C	3.92
C5	276-LEU	CD1	4.05
C19	276-LEU	CD1	4.04
C7	276-LEU	CD2	4.09
C9	276-LEU	CD2	3.95
C11	276-LEU	CD2	4.13
NI	276-LEU	CD2	4.17
C13	277-SER	N	4.14
C15	277-SER	N	3.79
C17	277-SER	N	3.69
N1	277-SER	N	3.30
O3	277-SER	N	3.19
C17	277-SER	CA	3.92
O3	277-SER	CA	3.35
C13	277-SER	OG	3.92
C7	287-LEU	CD2	3.90
C18	290-GLY	С	4.04
C18	290-GLY	0	3.54
C18	291-GLY	CA	4.04
C18	292-LEU	N	4.20
C2	292-LEU	CG	4.18
C4	292-LEU	CG	3.86
C6	292-LEU	CG	4.01
C2	292-LEU	CD1	3.88
C4	292-LEU	CD1	4.02
O2	292-LEU	CD1	4.07
C4	292-LEU	CD2	4.05
C6	292-LEU	CD2	3.72
C8	292-LEU	CD2	3.69
C10	292-LEU	CD2	3.98
O1	292-LEU	CD2	4.16
C20	299-ILE	CD1	3.87
C8	381-HIS	CD2	3.90
C10	381-HIS	CD2	3.84
O1	381-HIS	GO2	3.40
O1	381-HIS	CEI	3.72
C8	381-HIS	NE2	3.47
C10	381-HIS	NE2	3.51
01	381-HIS	NE2	2.64
C6	388-MET	CE	3.90
C8	401-PHE	CE1	4.19
O1	401-PHE	CE1	3.37

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Dimit	Amino Acid	Amino Acid	<u>Distance</u>
Atom	in full length α	Atom	A
C16	401-PHE	CZ	3.97
01	401-PHE	CZ	3.28
NI	502-H ₂ O	O1	3.35
O3	502-H ₂ O	O1	2.56
O3	503-H ₂ O	O1	3.13
04	503-H ₂ O	01	3.72
O4	504-H ₂ O	O1	2.72

Legend to Table 8. The table lists the interactions with Dimit (DMT). The column headings are as follows:

- #1 The atom of Dimit that interacts with the amino acid of the receptor. These are also numbered in Figure 32.
 - #2 The amino acid in the full length $rTR\alpha$ that interacts with the ligand.
 - #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
 - #4 The distance in Å between Dimit and the protein atom.

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Table 9

Triac	Amino Acid	Amino Acid	
Atom	in full length α	Atom	Distance Å
I1	218-PHE	0	3.52
<u> </u>	221-ILE	CD1	4.16
II	221-ILE	CG1	3.92
III	222-ILE	CA	4.15
I1	222-ILE	СВ	4.03
I1	222-ILE	CG1	3.92
C8	222-ILE	CD1	4.12
C10	222-ILE	CD1	3.77
C12	222-ILE	CD1	3.79
C13	225-ALA	СВ	4.17
C3	225-ALA	СВ	3.86
C10	256-MET	SD	3.45
C12	256-MET	SD	3.73
C10	256-MET	CE	3.66
C12	256-MET	CE	3.77
I3	256-MET	CE	3.89
C1	259-MET	0	3.93
C11	259-MET	0	3.24
O3	259-MET	0	4.09
C1	259-MET	CB	3.89
C13	259-MET	O	3.74
C14	259-MET	0	3.96
C1	259-MET	СВ	3.89
C11	259-MET	CB	3.68
C13	259-MET	CB	4.01
C11	259-MET	CA	4.13
C13	259-MET	CA	4.20
13	260-SER	CA	4.10
I3	260-SER	OG	4.19
C14	262-ARG	CB	4.07
04	262-ARG	СВ	3.60
O3	263-ALA	N	3.79
C14	263-ALA	N	4.12
O3	263-ALA	CA	3.67
O3	263-ALA	CB	3.49
C11	263-ALA	СВ	4.00
C14	266-ARG	CZ	3.89
03	266-ARG	CZ	4.01
04	266-ARG	CZ	3.03
C14	266-ARG	NH1	3.25
O3	266-ARG	NH1	3.00
04	266-ARG	NH1	2.82

Triac	Amino Acid	Amino Acid	Distance Å
Atom	in full length α	Atom	I
C14	266-ARG	NH2	3.48
03	266-ARG	NH2	4.01
04	266-ARG	NH2	2.34
03	275-THR	C	4.02
C14	275-THR	0	4.20
O3	275-THR	0	3.20
O3	278-LEU	CA	3.11
03	276-LEU	С	3.52
O3	276-LEU	N	4.04
C14	276-LEU	CA	3.98
O3	276-LEU	CA	3.11
C14	276-LEU	C	3.98
O3	276-LEU	СВ	3.95
O2	276-LEU	CD1	4.03
I1	276-LEU	CD1	4.10
C7	276-LEU	CD2	3.84
C9	276-LEU	CD2	3.73
CII	276-LEU	CD2	4.06
O2	276-LEU	CD2	4.10
03	276-LEU	CD2	3.91
C13	277-SER	N	4.06
C14	277-SER	N	3.13
O4	277-SER	N	3.28
O3	277-SER	N	3.05
C14	277-SER	CA	3.76
O4	277-SER	CA	3.52
C3	277-SER	OG	3.87
C13	277-SER	OG	4.02
C14	277-SER	OG	4.14
I2	290-GLY	0	3.57
I2	292-LEU	CG	3.94
C4	292-LEU	CG	3.95
C6	292-LEU	CG	3.65
C8	292-LEU	CG	4.02
C2	292-LEU	CD1	4.11
C4	292-LEU	CD1	3.85
C6	292-LEU	CD1	4.02
I2	292-LEU	CD2	3.98
C4	292-LEU	CD2	4.11
C6	292-LEU	CD2	3.44
C8	292-LEU	CD2	3.28
C10	292-LEU	CD2	3.88
01	292-LEU	CD2	3.35
I3	299-ILE	CD1	3.77

Triac	Amino Acid	Amino Acid	
Atom	in full length α	Atom	Distance Å
C8	381-HIS	CD2	3.87
C10	381-HIS	CD2	3.90
Ol	381-HIS	GO2	3.20
O1	381-HIS	CEI	3.82
C8	381-HIS	NE2	3.57
C10	381-HIS	NE2	3.52
O1	381-HIS	NE2	2.64
01	388-MET	CE	4.03
01	401-PHE	CE1	3.86
01	401-PHE	CZ	3.70
C13	460-H ₂ 0	01	4.00

Legend to Table 9. The table lists the interactions with Triac. The column headings are as follows:

- #1 The atom of Triac that interacts with the amino acid of the receptor. These are also 5 numbered in Figure 32.
 - #2 The amino acid in the full length rTRa that interacts with the ligand.
 - #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
 - #4 The distance in Å between Triac and the protein atom.

Table 10

IpBR ₂ Atom	Amino Acid	Amino Acid	Distance
1p2142 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	in full length α	Atom	Å
C16	215-PHE	CD1	4.01
C16	215-PHE	CEI	3.78
BR1	218-PHE	0	3.24
BR1	218-PHE	C	3.98
C16	218-PHE	СВ	3.81
C18	218-PHE	СВ	3.92
BR1	218-PHE	СВ	4.08
C18	218-PHE	CD2	3.92
C16	219-THR	CG2	3.45
BR1	221-ILE	CG1	3.81
BR1	221-ILE	CD1	4.07
BR1	222-ILE	СВ	3.81
BR1	222-ILE	CG1	3.97
<u>C6</u>	222-ILE	CD1	4.07
C8	222-ILE	CD1	3.64
C10	222-ILE	CD1	3.50
C12	222-ILE	CD1	3.82
01	222-ILE	CD1	4.08
C13	225-ALA	СВ	3.76
04	225-ALA	СВ	4.01
04	228-ARG	CZ	3.92
C17	228-ARG	NH2	3.26
03	228-ARG	NH2	3.43
04	228-ARG	NH2	2.79
C10	256-MET	SD	3.65
C12	256-MET	SD	3.71
C10	256-MET	CE	3.90
C12	256-MET	CE	3.75
BR2	256-MET	CE	4.03
C11	259-MET	C	3.98
C11	259-MET	0	3.52
C15	259-MET	0	3.44
NI	259-MET	0	3.76
C11	259-MET	СВ	3.87
NI	262-ARG	С	4.03
C15	262-ARG	СВ	4.03
C17	262-ARG	СВ	3.56
03	262-ARG	СВ	3.55
04	262-ARG	СВ	3.91
C17	262-ARG	CD	4.09
04	262-ARG	CD	3.71
NI	263-ALA	N	3.61

IpBR ₂ Atom	Amino Acid	Amino Acid	Distance
•	in full length α	Atom .	Å
NI	263-ALA	CA	3.59
N1	263-ALA	СВ	3.54
03	266-ARG	NH1	3.93
N1	275-THR	0	3.43
N1	276-LEU	CA	3.46
NI	276-LEU	C	3.83
C5	276-LEU	CD1	4.02
C7	276-LEU	CD2	4.00
C9	276-LEU	CD2	3.81
C11	276-LEU	CD2	3.91
C13	277-SER	N	3.79
C15	277-SER	N	3.63
C17	277-SER	N	3.70
N1	277-SER	N	3.17
03	277-SER	N	3.37
C17	277-SER	CA	3.89
03	277-SER	CA	3.43
C13	277-SER	OG	3.66
02	287-LEU	CD1	4.05
C18	290-GLY	C	4.04
C18	290-GLY	0	3.48
C18	291-GLY	CA	4.02
C4	292-LEU	CG	3.89
C6	292-LEU	CG	4.02
C2	292-LEU	CD1	3.79
C4	292-LEU	CD1	3.96
02	292-LEU	CD1	3.97
C4	292-LEU	CD2	4.07
C6	292-LEU	CD2	3.75
C8	292-LEU	CD2	3.67
C10	292-LEU	CD2	3.92
BR2	299-ILE	CD1	3.68
C8	381-HIS	CD2	3.92
C10	381-HIS	CD2	3.78
01	381-HIS	GD2	3.50
01	381-HIS	CE1	3.62
C8	381-HIS	NE2	3.36
C10	381-HIS	NE2	3.34
01	381-HIS	NE2	2.62
C8	401-PHE	CE1	4.02
01	401-PHE	CE1	3.19
C16	401-PHE	CZ	4.03
01	401-PHE	CZ	3.06
03	502-H ₂ O	01	3.40

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IpBR ₂ Atom	Amino Acid	Amino Acid	Distance
•	in full length α	Atom	Å
NI	502-H20	01	3.12
04	503-H ₂ O	01	3.20
C17	503-H20	01	3.04
03	503-H ₂ O	01	2.27
C15	504-H20	01	4.01
C17	504-H ₂ O	01	2.99
03	504-H2O	01	3.80
04	504-H ₂ O	01	1.78

Legend to Table 10. The table lists the interactions with IpBr2. The column headings are as follows:

- #1 The atom of IpBr2 that interacts with the amino acid of the receptor. These are also 5 numbered in Figure 32.
 - #2 The amino acid in the full length rTR α that interacts with the ligand.
 - #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
 - #4 The distance in Å between IpBr2 and the protein atom.

Table 11

Distance A
4.08 3.19 3.99 4.04 3.79 3.99 4.01 3.95 3.91
3.19 3.99 4.04 3.79 3.99 4.01 3.95 3.91
3.99 4.04 3.79 3.99 4.01 3.95 3.91
4.04 3.79 3.99 4.01 3.95 3.91
3.79 3.99 4.01 3.95 3.91
3.99 4.01 3.95 3.91
4.01 3.95 3.91
3.95 3.91
3.91
2 00
J.77
3.57
3.68
3.66
4.04
3.23
3.45
3.54
3.90
2.86
3.73
3.90
3.97
3.92
3.89
3.95
3.59
3.51
3.88
4.06
3.77
3.96
3.61
4.02
3.65
3.92
3.72
3.81
3.81
3.63
3.54
3.38
3.73
4.00

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T3 Atom	Amino Acid	Amino Acid	Distance
	in full length α	Atom	Å
C7	276-LEU	CD1	4.05
02	276-LEU	CD1	4.03
C7	276-LEU	CD2	3.80
C9	276-LEU	CD2	3.70
C11	276-LEU	CD2	4.01
C14	277-SER	N	3.67
C15	277-SER	N	3.62
N1	277-SER	N	3.07
03	277-SER	N	3.24
C15	277-SER	CA	3.77
03	277-SER	CA	3.34
C13	277-SER	OG	3.92
12	290-GLY	0	3.50
C4	292-LEU	CG	3.95
C8	292-LEU	CG	3.83
C2	292-LEU	CD1	4.07
C4	292-LEU	CD1	3.99
C4	292-LEU	CD2	4.09
C6	292-LEU	CD2	3.58
C8	292-LEU	CD2	3.50
C10	292-LEU	CD2	3.96
01	292-LEU	CD2	3.71
13	299-ILE	CD1	3.74
C8	381-HIS	CD2	3.94
C10	381-HIS	CD2	3.97
01	381-HIS	CD2	3.39
01	381-HIS	CD1	3.82
C8	381-HIS	NE2	3.47
C10	381-HIS	NE2	3.55
01	381-HIS	NE2	2.70
01	388-MET	CE	3.88
01	401-PHE	CE1	3.52
01	401-PHE	CZ	3.32
C14	502-H20	O1	4.01
C15	502-H2O	01	3.61
03	502-H20	01	2.51
C15	503-H2O	01	3.31
04	503-H ₂ O	01	3.10
N1	502-H ₂ O	01	3.27
03	503-H2O	01	2.81
C15	504-H2O	O1	3.92
04	504-H2O	01	2.73

Legend to Table 11. The table lists the interactions with T3. The column headings are as follows:

#1 The atom of T3 that interacts with the amino acid of the receptor. These are also numbered in Figure 32.

#2 The amino acid in the full length rTRα that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the 5 interaction occurs.

#4 The distance in Å between T3 and the protein atom.

Table 12

Triac	Amino Acid	Amino Acid	
Atom	in full length hTR β	Atom	Distance Å
I2	269-PHE	CD1	3.75
12	269-PHE	CE1	3.88
II	272-PHE	С	4.03
I1	272-PHE	0	3.54
<u> </u>	275-ILE	CG1	3.93
I1	276-ILE	CG1	4.02
C3	279-ALA	СВ	3.81
C13	279-ALA	СВ	3.87
C10	310-MET	SD	3.72
C12	310-MET	SD	3.78
C10	310-MET	CE	4.02
C12	310-MET	CE	3.92
I3	310-MET	CE	3.93
C13	313-MET	CA	3.94
C11	313-MET	C	3.72
Cl	313-MET	0	3.79
C11	313-MET	0	3.12
C13	313-MET	0	3.55
Cl	313-MET	CB	4.00
C11	313-MET	СВ	3.82
C13	313-MET	СВ	3.76
C13	313-MET	CG	3.88
O3	316-ARG	СВ	3.99
O4	317-ALA	CA	4.08
04	317-ALA	CA	4.10
C11	317-ALA	CB	3.70
I3	317-ALA	CB	4.10
O4	317-ALA	СВ	4.06
O4	320-ARG	NHI	3.58
03	320-ARG	NH2	3.55
04	320-ARG	NH2	4.04
04	329-THR	0	3.55
04	330-LEU	CA	3.42
04	330-LEU	C	3.77
C3	330-LEU	СВ	4.06
C5	330-LEU	СВ	4.08
Cl	330-LEU	CD2	4.07
C3	330-LEU	CD2	4.00
C5	330-LEU	CD2	3.73
C7	330-LEU	CD2	3.51
C9	330-LEU	CD2	3.54
C11	330-LEU	CD2	3.86

Triac	Amino Acid	Amino Acid	_
Atom	in full length hTR β	Atom	Distance Å
C15	331-ASN	N	3.55
O3	331-ASN	N	3.74
O4	331-ASN	N	3.12
03	331-ASN	CA	4.02
I2	344-GLY	0	3.87
C6	346-LEU	CD2	3.87
C8	346-LEU	CD2	3.84
01	346-LEU	CD2	3.91
I3	353-ILE	CD1	3.51
C8	435-HIS	CD2	3.93
C10	435-HIS	CD2	3.79
01	435-HIS	CD2	3.33
01	435-HIS	CE1	3.81
C8	435-HIS	NE2	3.42
C10	435-HIS	NE2	3.33
01	435-HIS	NE2	2.67
01	442-MET	SD	3.96
01	442-MET	CE	3.72
I2	442-MET	SD	4.01
O1	455-PHE	CE1	3.92
O1	455-PHE	CZ	3.50

Legend to Table 12. The table lists the interactions with Triac. The column headings are as follows:

^{#1} The atom of Triac that interacts with the amino acid of the receptor. These are also 5 numbered in Figure 32.

^{#2} The amino acid in the full length $hTR\beta$ that interacts with the ligand.

^{#3} The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

^{#4} The distance in Å between Triac and the protein atom.

Table 13

GC1	Amino Acid	Amino Acid	
Atom	in full length TR β	Atom	Distance Å
C16	269-PHE	CE1	3.99
C19	272-PHE	0	3.85
C16	272-PHE	CB	3.98
C16	273-THR	CG2	3.76
C19	275-ILE	CG1	3.98
C19	276-ILE	CA	3.98
C2	276-ILE	CD1	3.88
C8	276-ILE	CD1	3.77
C10	276-ILE	CD1	3.58
C12	276-ILE	CD1	3.62
C19	276-ILE	CD1	3.56
Cl	279-ALA	СВ	3.68
C3	279-ALA	СВ	3.56
O5	279-ALA	CB	3.11
04	279-ALA	СВ	3.90
O3	282-ARG	CZ	3.53
C17	282-ARG	NHI	3.87
O3	282-ARG	NH1	3.20
04	282-ARG	NH1	3.85
C17	282-ARG	NH2	3.63
O3	282-ARG	NH2	3.00
C10	310-MET	SD	3.86
C12	310-MET	SD	3.91
C11	313-MET	С	3.85
C11	313-MET	0	3.41
C15	313-MET	0	3.87
C20	313-MET	0	3.99
C11	313-MET	CB	3.79
C1	313-MET	CG	3.94
C11	313-MET	CG	3.91
O5	313-MET	CG	3.87
O4	313-MET	CG	3.79
C20	314-SER	CA	4.00
C17	316-ARG	CB	3.95
C17	316-ARG	CD	3.80
O3	316-ARG	CD	3.83
O4	316-ARG	CD	3.51
C20	317-ALA	СВ	3.93
C7	330-LEU	CD2	3.56
C9	330-LEU	CD2	3.63
C21	330-LEU	CD2	3.90
O5	331-ASN	N	3.62

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GC1	Amino Acid	Amino Acid	_
Atom	in full length TR β	Atom	Distance Å
C15	331-ASN	N	3.67
C18	344-GLY	0	3.60
C18	346-LEU	CG	3.89
C6	346-LEU	CD2	3.77
C8	346-LEÚ	CD2	3.80
C10	435-HIS	CD2	3.89
01	435-HIS	CD2	3.64
O1	435-HIS	CE1	3.79
C8	435-HIS	NE2	3.44
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.77
O1	455-PHE	CE1	3.40
O1	455-PHE	CZ	3.22

Legend to Table 13. The table lists the interactions with GC1. The column headings are as follows:

- #1 The atom of GC1 that interacts with the amino acid of the receptor. These are also 5 numbered in Figure 32.
 - #2 The amino acid in the full length hTRβ that interacts with the ligand.
 - #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
 - #4 The distance in Å between GC1 and the protein atom.

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PCT/US98/25296

Structure		Coo	rdina	ation S	tructu	re of T	'R-α	and Din	rit			
CHp-CH(NH,)(CO,)H	Coordina-	R ₁	R ₂	R ₃	R ₅	R ₆	R'2	R'3	R' ₄	R's	R'6	Х
Structure		.	-	_	,		_					
AA												
SS		-CH2-CH(NH2)(CO2)H	-H	-CH ₃	-CH ₃	-H	-H		-OH	-H	-H	0
SS	AA			1				215				
AA	SS			T				Н3				
SS				218				218				
AA	SS	-	-	Н3				Н3				
SS					i			219				
AA	SS			 				Н3				
SS				221								
AAA	SS			H3								
SS H3 H5 H6 H5-H6 H5-H6 H5-H6 H5-H6 H5-H6 H5-H6 H5-H6 H5-H6 H6 H6-H5-H6 H6-H5-H6 <td< td=""><td></td><td></td><td>-</td><td><u> </u></td><td></td><td></td><td></td><td>222</td><td>222</td><td></td><td>222</td><td></td></td<>			-	<u> </u>				222	222		222	
AA	SS							H3	H3	H3	H3	
SS				1				1				
AA 228	SS	H3		1		1						
SS H3 256 256 SS H5-H6		228										
AA	SS	H3		†	1							
SS 4AA 259 259 H5-H6 H5-H6 <td></td> <td> </td> <td></td> <td>1</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>256</td> <td>256</td> <td></td>				1						256	256	
AA 259 SS H5-H6 AA 262 SS H5-H6 AA 263 SS H5-H6 AA 266 SS loop AA 275 SS S3 AA 276 SS S3 AA 277 SS loop AA 277 SS loop AA 277 SS loop AA 277 SS loop AA 278 SS loop AA 279 SS loop AA 277 SS loop AA 3 383 SS	SS	<u> </u>		1	1					H5-H6	H5-H6	
SS H5-H6 H5-H6 AA 262 SS SS H5-H6 SS AA 263 SS SS H5-H6 SS AA 266 SS SS Ioop SS AA 275 SS SS S3 S3 AA 276 276 276 SS S3 S3 S3 AA 277 SS Ioop AA 290-291 SS SS Ioop Ioop AA 292 292 292 SS Ioop Ioop Ioop AA 299 SS Intil H11 AA 388 SS AA 401 401 401 SS H12 H12 H12 AA H0H502/HOH503 H12 H12 H12				1								
SS H5-H6 AA 263 SS H5-H6 AA 266 SS loop AA 275 SS S3 AA 276 276 276 SS S3 S3 S3 AA 277 SS loop AA 290-291 SS SS loop loop AA 292 292 292 SS loop loop loop loop AA 381 381 SS H11 H11 AA 401 401 SS H12 H12 AA H12 H12		H5-H6		_	1	H5-H6						I
SS H5-H6 AA 263 SS H5-H6 AA 266 SS loop AA 275 SS S3 AA 276 276 276 SS S3 S3 S3 AA 277 SS loop AA 290-291 SS SS loop SS AA 292 292 292 SS loop loop loop loop AA 381 381 SS H11 H11 AA 401 401 SS H12 H12 AA H12 H12		262		1	1							
AA 263 SS H5-H6 AA 266 SS loop AA 275 SS S3 AA 276 276 276 276 SS S3 AA 277 SS loop AA 3 290-291 SS	SS	H5-H6			1	1	-					
SS H5-H6 AA 266 SS loop AA 275 SS S3 AA 276 276 276 SS S3 S3 S3 AA 277 SS loop AA 290-291 SS SS loop loop AA 292 292 292 SS loop loop loop loop loop AA 381 381 SS H11 H11 AA 388 SS H11 H11 H12 AA H01 H01 AA H01 H01		263										
AA 266 SS loop AA 275 SS S3 AA 276 276 276 276 SS S3 S3 S3 S3 S3 AA 277 SS loop AA 277 SS loop AA 277 SS loop AA 290-291 SS loop AA 299 292 292 292 292 SS H8 381 381 SS H8 388 SS SS H11 AA SSS H11 H11 H11 AA 4 401 401 SS H12 H12 H12 AA HOH502/HOH503	SS	H5-H6										
SS		266		T				1				
AA 275 SS S3 AA 276 276 276 276 SS S3 S3 S3 S3 S3 AA 277 SS loop AA 290-291 SS loop AA 292 292 292 292 SS loop loop loop loop loop AA 3 299 SS	SS	loop										
AA 276 276 276 276 58	AA	275										
SS S3 S4 S3 S4 S4<	SS		-	1								
AA 277 SS loop AA 290-291 SS loop AA 292 292 292 292 SS loop loop loop loop loop AA 299 SS H8 381 381 SS H11 H11 AA 388 SS H11 AA 401 401 SS H12 H12 AA HOH502/HOH503	AA						1					L
SS loop AA 290-291 SS loop AA 292 292 292 SS loop loop loop loop loop AA 299 381 381 SS H11 H11 H11 AA 388 SS AA 401 401 SS H12 H12 AA H0H502/HOH503 H12 H12	SS			S3	S3	S3						
AA		277							I			
SS loop AA 292 292 292 292 SS loop loop loop loop loop loop loop loop AA 299 381 381 381 SS H11 H11 H11 H11 AA 388 SS H11 H11 AA 401 401 SS H12 H12 AA H0H502/HOH503 H12 H12 H12 H12	SS	loop										
AA	AA										1	<u> </u>
SS	SS											
AA	AA						292		292		<u></u>	292
SS	SS						loop	loop	loop	loop		loop
AA 381 381 SS H11 H11 AA 388 SS H11 AA 401 401 SS H12 H12 AA H0H502/HOH503	AA								J			
SS					H8							
SS	AA										ļ	ļ
SS H11 AA 401 401 SS H12 H12 AA HOH502/HOH503	SS								HII	H11		1
AA	AA											<u> </u>
SS H12 H12 H2 AA HOH502/HOH503												
AA HOH502/HOH503								1				
	SS							H12	H12			
/HOH504	AA	HOH502/HOH503 /HOH504										
SS	SS				1		T					

AA = Amino Acid

SS = Secondary Structure

Coordination	R _I	R_2	R ₃	R ₅	R ₆	R'2	R'3	R'4	R'5	R'6	Х
Structure						<u> </u>			<u> </u>		
	-CH ₂ -COOH	-H	-I	-1	-H	-H	-I	-OH	-Н	-H	0
AA			218						<u> </u>	<u> </u>	ļ
SS	-		H3								
AA			221						<u> </u>	<u> </u>	
SS			H3					L	ļ	ļ	
AA							222	222	222	222	
SS							H3	H3	Н3	Н3	
AA	225										
SS	H3										<u> </u>
AA				256					256	256	
SS				H5-H6					H5-H6	H5-H6	
AA	259				259						
SS	H5-H6		T		H5-H6		l				
AA	262										
SS	H5-H6										L
AA	263										<u> </u>
SS	H5-H6										
AA	266		T								
SS	loop									<u> </u>	
AA	275										
SS	S3										
AA	276		276	276	276						<u></u>
SS	S3	1	S3	S3	S3	_1					
AA	277										
SS	loop										
AA							290			1	
SS						Ī	loop				
AA					Ī	292	292	292	292		292
SS			T			loop	loop	loop	loop		loop
AA				299							\bot
SS		1		H8							
AA		T						381	381		
SS		1						H11	H11		
AA		1						388			1
SS		1						H11			
AA		1	7				401	401			
SS		1					H12	H12			

5 AA = Amino Acid SS = Secondary Structure

Table 16
Coordination Structure of TR-α and IpBr2

					cture of	I'R-α	and IpB	r2			
Coordina- tion Structure	R ₁	R ₂	R ₃	R ₅	R ₆	R'2	R'3	R' ₄	R'5	R'6	X
Suuctuic	-CH ₂ -CH(NH ₂)(CO ₂)H	-H	-Br	-Br	-H	-H	-CH(CH ₁) ₂	-OH	-H	-H	0
ĀĀ	, , ,, ,,						215	-			
SS					-		H3				
AA			218				218				
SS	-	-	Н3				Н3				
AA							219				
SS							Н3				
AA			221								
SS			Н3								
AA							222	222	222	222	
SS							Н3	H3	H3	H3	
AA	225										
SS	Н3										
AA	228									<u> </u>	
SS	H3		<u> </u>					ļ			
AA					256		<u> </u>	<u> </u>	256	256	<u> </u>
SS					H5-H6			ļ	H5-H6	Н5-Н6	<u> </u>
AA	259				259	<u> </u>	ļ	 		ļ	<u> </u>
SS	Н5-Н6	<u> </u>			H5-H6	ļ		ļ		ļ	
AA	262	ļ	ļ			<u> </u>		<u> </u>	ļ	 	
SS	H5-H6		ļ			<u> </u>		ļ			├
AA	263		 			ļ				 	ļ
SS	H5-H6	ļ	 					-		 	
SS S	266	 	-				<u> </u>	1		ļ	
	loop 275	 				 	 	 		-	
SS S	S3	ļ	 			 				 	
AA	276	<u> </u>	276	276	276	 		 	 -	 	+
SS	S3	 	S3	S3	S3	 	ļ. — —	 	 		1
AA	277	1	+ 55	33	55	 			 	1	† · · ·
SS	211	 	+		 	 	+	 	 	1	1
AA	 	 	 	 		 	290-291		1		1
SS		 	+	ļ	 	 	loop	1		 	
AA		+			+	292	292	292	292		292
SS	 	1	1	†		loop	loop	loop	loop		loop
AA		1	1	299		1		1			
SS	1			H8		T					
AA	<u> </u>	1	1		† · · · · ·			381	381		
SS		1	 	1	†	1		HII	H11		
AA		1	1	1	T	1	401	401			
SS		1		1	T		H12	H12			
AA	HOH502/HOH503/ HOH504										
SS		1			<u> </u>	C			<u></u>		Т

AA = Amino Acid

SS = Secondary Structure

Table 17
Coordination Structure of TR-α and Dimit

Coordination	R ₁	R ₂	R ₃	R ₅	e of TR	R'2	R' ₃	R' ₄	R's	R'6	X
Structure	K ₁	12	103	***	***	2	,		,		
Structure	-CH ₂ -CH(NH ₂)(CO ₁)H	-H	-1	-1	-H	-H	-I	-ОН	-H	-H	0
AA .	 		1				215				
SS	 						H3				
AA .	 		218			218					-
SS			H3			H3					
AA	+		221								
SS	 		Н3							<u></u>	
AA	 		1				222	222	222	222	
SS	 		1				H3	H3	H3	H3	
AA	225					-					
SS	H3		 					_			
ĀĀ	228		+		·						
SS	H3		+								
AA		l	 		256				256	256	
SS			 		H5-H6				H5-H6	H5-H6	
ĀĀ	259		†···		259						
SS	Н5-Н6	<u> </u>	 		H5-H6						
AA	262										
SS	H5-H6	1	1		†						
AA	263	†	T			1					
SS	H5-H6	 									
AA	275		T								
SS	S3		1	1						<u> </u>	Ì
AA	276		276	276	276						<u> </u>
SS	S3		S3	S3	S3						<u> </u>
ĀĀ	277								<u></u>		
SS											
AA							290	<u></u>			
SS				1			loop				
AA				Ţ		292	292	292	292		292
SS						loop	loop	loop	loop	<u> </u>	loop
AA				299		I		ļ		_	
SS				H8					<u> </u>	ļ	
AA				}				381	381	-	
SS								H11	H11	 	
AA								388			
SS							1	H11		 	-
AA							401	401		 	
SS							H12	H12	1	+	
AA SS	HOH502/H0H503/ HOH504								<u> </u>		

AA = Amino Acid SS = Secondary Structure

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Table 18
Coordination Structure of TR-β and Triac

Coordination	Ri	R2	R3	R5	R6	R2'	R3	R4	R5	R6	X
Structure					77	;-	-	ОН	н	н	O
	-CH ₂ CO ₂ H	Н	I	I	Н	Н	1	OH	-H	n	
AA							269				
SS							Н3				
AA			272		•						
SS	<u> </u>		H3								
AA	<u> </u>		275								
SS			Н3			ļ					
AA			276			L					
SS			H3			L					
AA	279	279									
SS	H3	Н3									
AA				310					310	310	
SS				H5-H6					H5-H6	H5-H6	
AA	313				313						
SS	H5-H6				H5-H6						
AA	316	1									
SS	H5-H6		· · ·								
AA	317				317		317				
SS	H5-H6	1			H5-H6	1	H5-H6				
AA	320										
SS	H5-H6		<u> </u>								
AA	329		 		· · · · · · · · · · · · · · · · · · ·						
SS	S3				<u> </u>	1					
AA	330	330	330	330	330						
SS	S3	S3	S3	S3	S3	1					
AA	331		1								
SS	loop	1	1	1		1	1	1			
AA	- 	 		1	1	1	344				
SS	·	1	†	1		1	loop				
AA		1~					346	346			
SS		1	1	1	1	1	loop	loop			T
AA		+	- 	353		—	<u> </u>	1	T	Ī	T
SS	 	1	1	H8				T	1		
AA	 	1	1	1	 	\top		435	435	1	
SS		+	1	 	1	_		HII	H11	1	1
AA		 	+		 	+-	442	442		T	1
SS	 	+	+		 	+	HII	HII	1		1
AA			+	 	+	 		455	1		1
SS		+	+	 	+		 	H12		 	\top

AA = Amino Acid

SS = Secondary Structure

Table 19
Coordination Structure of TR-β and GC1

							β and GC				
Coordina-	R ₁	R ₂	R ₃	R5	R ₆	R2	R3	R4	R5	R6	Х
ion							(
Structure											
	-O-CH ₂ CO ₂ H	Н	CH ₃	CH ₃	Н	Н	CH(CH ₃)	OH	H	Н	CH ₂
ĀĀ							269				
SS							H3				
AA			272								
SS			H3								
AA			273				273				
SS			H3				Н3				
AA	1		275	i .							
SS			H3								
AA			276					276	276	276	
SS			H3					H3	H3	H3	
AA	279	279									
SS	H3	H3									
AA SS	282										
SS	H3										
AA				310					310	310	ļ
SS	Ì			H5-H6					H5-	H5-H6	
			1			l	İ		Н6		<u> </u>
AA	313				313						
SS	H5-H6				H5-H6	Ī					
AA							314			<u> </u>	
SS							H5-H6	<u> </u>			
AA SS	316	1						<u> </u>			<u> </u>
SS	H5-H6		1								<u> </u>
AA							317	<u> </u>		1	ļ
SS							H5-H6				<u> </u>
AA	320										<u> </u>
SS	H5-H6								<u></u>		
AA	329										
SS	S3										
AA	330			330					<u> </u>		
SS	S3			S3				<u> </u>	ļ		1
AA	331								ļ		
SS	loop							ļ	<u> </u>	ļ	↓—
AA							344		ļ	ļ	1
SS							loop	1	<u> </u>	<u> </u>	\bot
AA							346	346		<u> </u>	\perp
SS							loop	loop	ļ		↓
AA				353				1	L		
SS				H8							
AA					I			435	435	1	4
		1						HII	H11		
								455			
SS								H12	1	1	1

AA = Amino Acid

SS = Secondary Structure

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PCT/US98/25296

N.D.ZILZ,

APPENDIX 3

TR_DMT.PDB

REMARK TR_dmt full length numbering

REMARK

5 REMARK Rfactor 0.205 Rfree 0.227

REMARK Resolution 15. 2.2 all reflections

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392

10 REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

15 REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

REMARK 281 Thr - Ala

20 REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY,

N.L.MCCREARY, M.J.MACDONALD

25 JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES FOR TWO

JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC

45

V. 263 25 1988

30 JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE

V. 237 1987

35 JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE TRANSCRIPT

40 JRNL REF NUC. ACIDS. RES. V. 16 12 1988

ATOM 1 N ARG 157 68.504 8.445 5.651 1.00 68.93

ATOM 2 CA ARG 157 67.886 9.543 6.398 1.00 56.98

ATOM 3 CB ARG 157 68.769 10.789 6.324 1.00 59.25

ATOM 4 CG ARG 157 70.147 10.632 6.932 1.00 58.90

ATOM 5 CD ARG 157 70.068 10.422 8.425 1.00 59.37

ATOM 6 NE ARG 157 71.392 10.446 9.036 1.00 63.94

ATOM 7 CZ ARG 157 71.613 10.329 10.341 1.00 64.39

ATOM 8 NH1 ARG 157 70.596 10.182 11.179 1.00 62.14

```
72.855 10.365 10.808 1.00 65.56
             9 NH2 ARG 157
    ATOM
    ATOM
            10 C ARG 157
                              66.500 9.881 5.854 1.00 48.97
            11 O ARG 157
                              66.351 10.203 4.674 1.00 48.61
    ATOM
            12 N PRO 158
                             65.469 9.818 6.712 1.00 41.90
    ATOM
                              65.550 9.366 8.112 1.00 41.06
            13 CD PRO 158
    ATOM
                              64.083 10.114 6.333 1.00 39.34
            14 CA PRO 158
    ATOM
                              63.286 9.704 7.576 1.00 37.89
            15 CB PRO 158
    ATOM
            16 CG PRO 158
                             64.260 9.883 8.693 1.00 42.40
    ATOM
            17 C PRO 158
                             63.814 11.573 5.930 1.00 37.10
    ATOM
            18 O PRO 158
                             64.189 12.517 6.636 1.00 33.31
10
    ATOM
                              63.171 11.733 4.778 1.00 30.56
    ATOM
            19 N GLU 159
                              62.821 13.038 4.231 1.00 24.26
    ATOM
            20 CA GLU 159
            21 CB GLU 159
                              62.553 12.904 2.727 1.00 19.19
    ATOM
            22 CG GLU 159
                              63.788 12.677 1.874 1.00 20.60
    ATOM
                              64.407 13.971 1.390 1.00 26.54
            23 CD GLU 159
    ATOM
15
                               63.649 14.929 1.115 1.00 30.85
            24 OE1 GLU 159
    ATOM
                               65.649 14.027 1.268 1.00 28.35
            25 OE2 GLU 159
    ATOM
                              61.549 13.520 4.909 1.00 23.26
            26 C GLU 159
    ATOM
            27 O GLU 159
                              60.906 12.765 5.643 1.00 26.86
    ATOM
                              61.200 14.806 4.729 1.00 22.72
20
    ATOM
            28 N PRO 160
                              61.981 15.916 4.153 1.00 17.87
    ATOM
            29 CD PRO 160
                              59.969 15.292 5.359 1.00 19.90
    ATOM
            30 CA PRO 160
             31 CB PRO 160
                              60.004 16.799 5.070 1.00 14.42
    ATOM
             32 CG PRO 160
                             61.465 17.109 4.919 1.00 12.87
    ATOM
            33 C PRO 160
                              58.747 14.623 4.701 1.00 23.68
    ATOM
25
                             58.730 14.383 3.491 1.00 24.72
            34 O PRO 160
    ATOM
                             57.749 14.281 5.506 1.00 22.19
            35 N THR 161
    ATOM
                              56.542 13.660 4.985 1.00 19.50
            36 CA THR 161
    ATOM
                               55.691 13.031 6.125 1.00 21.50
            37 CB THR 161
    ATOM
                               55.163 14.062 6.972 1.00 20.33
            38 OG1 THR 161
30
    ATOM
                               56.537 12.078 6.959 1.00 19.48
            39 CG2 THR 161
    ATOM
                              55.744 14.765 4.298 1.00 22.86
    ATOM
             40 C THR 161
                              56.040 15.949 4.481 1.00 27.68
             41 O THR 161
    ATOM
             42 N PRO 162
                              54.720 14.403 3.504 1.00 20.36
    ATOM
             43 CD PRO 162
                               54.280 13.050 3.113 1.00 16.55
35
    ATOM
                               53.924 15.435 2.830 1.00 21.97
             44 CA PRO 162
     ATOM
                               52.780 14.633 2.210 1.00 18.17
             45 CB PRO 162
     ATOM
            46 CG PRO 162
                             53.422 13.316 1.905 1.00 18.01
     ATOM
            47 C PRO 162
                             53.399 16.467 3.826 1.00 22.56
     ATOM
                              53.461 17.675 3.567 1.00 21.73
            48 O PRO 162
40
     ATOM
                              52.912 15.976 4.967 1.00 25.28
             49 N GLU 163
     ATOM
                              52.357 16.816 6.030 1.00 26.64
     ATOM
             50 CA GLU 163
                               51.743 15.962 7.144 1.00 30.22
             51 CB GLU 163
     ATOM
             52 CG GLU 163
                               50.514 15.131 6.748 1.00 44.99
     ATOM
                               50.836 13.950 5.831 1.00 48.88
             53 CD GLU 163
    ATOM
45
                               50.016 13.660 4.929 1.00 52.48
             54 OE1 GLU 163
     ATOM
                               51.895 13.309 6.015 1.00 44.23
             55 OE2 GLU 163
     ATOM
            56 C GLU 163
                              53.414 17.731 6.634 1.00 27.65
     ATOM
                              53.114 18.862 7.034 1.00 29.30
             57 O GLU 163
     ATOM
                              54.646 17.235 6.712 1.00 21.89
            58 N GLU 164
50
     ATOM
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	ATOM	59 CA GLU 164	55.741 18.015 7.265 1.00 18.29
	ATOM	60 CB GLU 164	56.901 17.109 7.657 1.00 14.78
	ATOM	61 CG GLU 164	56.552 16.196 8.825 1.00 21.11
	ATOM	62 CD GLU 164	57.669 15.249 9.198 1.00 20.35
5	ATOM	63 OE1 GLU 164	58.605 15.071 8.392 1.00 28.55
_	ATOM	64 OE2 GLU 164	57.610 14.677 10.302 1.00 28.25
	ATOM	65 C GLU 164	56.200 19.097 6.306 1.00 24.62
	ATOM	66 O GLU 164	56.574 20.183 6.741 1.00 32.05
	ATOM	67 N TRP 165	56.174 18.817 5.003 1.00 28.22
10	ATOM	68 CA TRP 165	56.576 19.825 4.021 1.00 22.99
10	ATOM	69 CB TRP 165	56.575 19.262 2.605 1.00 17.37
	ATOM	70 CG TRP 165	57.876 18.633 2.210 1.00 10.74
	ATOM	71 CD2 TRP 165	59.153 19.283 2.109 1.00 11.74
		72 CE2 TRP 165	60.075 18.319 1.648 1.00 9.97
1.5	ATOM	73 CE3 TRP 165	59.606 20.583 2.365 1.00 13.88
15	ATOM	74 CD1 TRP 165	58.074 17.343 1.832 1.00 9.17
	ATOM		59.390 17.145 1.486 1.00 16.55
	ATOM		61.427 18.613 1.436 1.00 13.37
	ATOM	76 CZ2 TRP 165	60.954 20.874 2.156 1.00 16.15
	ATOM	77 CZ3 TRP 165	
20	ATOM	78 CH2 TRP 165	
	ATOM	79 C TRP 165	
	ATOM	80 O TRP 165	201011
	ATOM	81 N ASP 166	
	ATOM	82 CA ASP 166	
25	ATOM	83 CB ASP 166	* · · ·
	ATOM	84 CG ASP 166	
	ATOM	85 OD1 ASP 166	
	ATOM	86 OD2 ASP 166	
	ATOM	87 C ASP 166	53.732 22.637 5.842 1.00 27.91
30	ATOM	88 O ASP 166	53.744 23.865 5.767 1.00 31.28
	ATOM	89 N LEU 167	54.046 21.966 6.951 1.00 25.57
	ATOM	90 CA LEU 167	54.439 22.640 8.187 1.00 28.28
	ATOM	91 CB LEU 167	54.854 21.624 9.256 1.00 32.80
	ATOM	92 CG LEU 167	53.945 21.347 10.455 1.00 41.75
35	ATOM	93 CD1 LEU 167	54.765 20.640 11.532 1.00 39.15
	ATOM	94 CD2 LEU 167	53.374 22.647 11.008 1.00 39.20
	ATOM	95 C LEU 167	55.636 23.532 7.902 1.00 22.19
	ATOM	96 O LEU 167	55.671 24.700 8.302 1.00 29.51
	ATOM	97 N ILE 168	56.610 22.957 7.206 1.00 15.01
40	ATOM	98 CA ILE 168	57.846 23.632 6.833 1.00 18.03
	ATOM	99 CB ILE 168	58.756 22.668 6.040 1.00 11.37
	ATOM	100 CG2 ILE 168	59.890 23.413 5.367 1.00 16.36
	ATOM	101 CG1 ILE 168	59.289 21.580 6.975 1.00 21.63
	ATOM	102 CD1 ILE 168	60.095 20.501 6.287 1.00 21.03
45	ATOM	103 C ILE 168	57.579 24.897 6.022 1.00 22.54
	ATOM	104 O ILE 168	58.155 25.948 6.300 1.00 24.88
	ATOM	105 N HIS 169	56.682 24.800 5.045 1.00 25.70
	ATOM	106 CA HIS 169	56.337 25.934 4.190 1.00 21.28
	ATOM	107 CB HIS 169	55.411 25.493 3.057 1.00 22.29
50	ATOM	108 CG HIS 169	56.047 24.543 2.091 1.00 23.11

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ATOM

57.348 24.265 1.839 1.00 16.86 ATOM 109 CD2 HIS 169 55.312 23.721 1.263 1.00 25.30 ATOM 110 ND1 HIS 169 56.130 22.974 0.546 1.00 15.89 ATOM 111 CE1 HIS 169 57.371 23.283 0.878 1.00 25.38 112 NE2 HIS 169 ATOM 113 C HIS 169 55.664 27.048 4.976 1.00 18.32 ATOM 56.033 28.215 4.842 1.00 21.53 114 O HIS 169 ATOM 54.679 26.685 5.795 1.00 17.13 115 N VAL 170 ATOM 53.957 27.661 6.607 1.00 21.29 116 CA VAL 170 ATOM 52.808 26.991 7.399 1.00 24.33 117 CB VAL 170 ATOM 52.164 27.985 8.354 1.00 23.78 118 CG1 VAL 170 10 ATOM 51.760 26.439 6.435 1.00 18.87 ATOM 119 CG2 VAL 170 54.910 28.382 7.567 1.00 24.69 ATOM 120 C VAL 170 121 O VAL 170 54.912 29.616 7.637 1.00 28.77 ATOM 55.759 27.609 8.245 1.00 20.35 122 N ALA 171 ATOM 56.722 28.148 9.202 1.00 19.61 123 CA ALA 171 ATOM 15 57.393 27.013 9.977 1.00 17.52 124 CB ALA 171 ATOM 57.775 29.026 8.531 1.00 20.91 125 C ALA 171 ATOM 126 O ALA 171 58.102 30.105 9.041 1.00 21.98 ATOM 127 N THR 172 58.308 28.571 7.398 1.00 18.94 ATOM 59.313 29.342 6.668 1.00 19.55 128 CA THR 172 20 ATOM 59.820 28.594 5.413 1.00 20.49 ATOM 129 CB THR 172 60.394 27.336 5.795 1.00 20.66 ATOM 130 OG1 THR 172 60.894 29.418 4.702 1.00 20.44 ATOM 131 CG2 THR 172 58.730 30.697 6.254 1.00 23.26 132 C THR 172 ATOM 133 O THR 172 59.403 31.724 6.334 1.00 24.32 ATOM 25 57.468 30.694 5.836 1.00 27.42 134 N GLU 173 ATOM 56.797 31.922 5.434 1.00 27.68 135 CA GLU 173 ATOM 55.477 31.605 4.728 1.00 24.51 136 CB GLU 173 ATOM 54.652 32.836 4.338 1.00 39.69 137 CG GLU 173 ATOM 138 CD GLU 173 55.396 33.814 3.426 1.00 47.72 ATOM 30 55.019 35.009 3.417 1.00 48.26 ATOM 139 OE1 GLU 173 56.344 33.398 2.717 1.00 49.61 140 OE2 GLU 173 ATOM 56.557 32.834 6.641 1.00 25.68 141 C GLU 173 ATOM ATOM 142 O GLU 173 56.773 34.046 6.559 1.00 23.39 56.119 32.245 7.755 1.00 25.19 143 N ALA 174 **ATOM** 35 144 CA ALA 174 55.863 32.989 8.993 1.00 22.25 **ATOM** 55.450 32.030 10.111 1.00 15.95 145 CB ALA 174 ATOM 57.125 33.747 9.391 1.00 23.22 146 C ALA 174 ATOM 57.076 34.918 9.768 1.00 24.52 **ATOM** 147 O ALA 174 58.261 33.073 9.275 1.00 20.97 148 N HIS 175 40 **ATOM** 149 CA HIS 175 59.544 33.665 9.606 1.00 19.55 **ATOM** 60.625 32.577 9.649 1.00 16.19 150 CB HIS 175 **ATOM** -62.016 33.104 9.835 1.00 18.89 ATOM 151 CG HIS 175 63.148 32.901 9.119 1.00 16.05 ATOM 152 CD2 HIS 175 62.359 33.962 10.859 1.00 13.83 153 ND1 HIS 175 ATOM 45 154 CE1 HIS 175 63.642 34.265 10.765 1.00 15.87 ATOM 64.143 33.635 9.718 1.00 19.19 155 NE2 HIS 175 **ATOM** 59.934 34.757 8.617 1.00 21.28 156 C HIS 175 ATOM 60.274 35.869 9.014 1.00 25.12 157 O HIS 175 ATOM 59.891 34.436 7.329 1.00 26.73 158 N ARG 176

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60.266 35.387 6.292 1.00 27.13
    ATOM
            159 CA ARG 176
                                60.156 34.748 4.914 1.00 36.00
            160 CB ARG 176
    ATOM
            161 CG ARG 176
                                61.286 33.795 4.602 1.00 43.20
    ATOM
                                61.197 33.334 3.170 1.00 50.07
            162 CD ARG 176
    ATOM
                                62.316 32.477 2.813 1.00 58.20
            163 NE ARG 176
    ATOM
                                62.266 31.548 1.867 1.00 67.22
            164 CZ ARG 176
    ATOM
                                61.143 31.358 1.182 1.00 67.62
    ATOM
            165 NH1 ARG 176
                                63.336 30.806 1.612 1.00 70.56
            166 NH2 ARG 176
    ATOM
                               59.487 36.688 6.325 1.00 23.97
    ATOM
            167 C ARG 176
                               60.073 37.760 6.209 1.00 24.52
10
    ATOM
            168 O ARG 176
                              58.177 36.598 6.515 1.00 23.60
    ATOM
            169 N SER 177
            170 CA SER 177
                               57.341 37.789 6.565 1.00 26.36
    ATOM
            171 CB SER 177
                               55.865 37.407 6.439 1.00 21.93
    ATOM
                              55.495 36.459 7.423 1.00 25.97
57.557 38.623 7.829 1.00 28.76
            172 OG SER 177
    ATOM
            173 C SER 177
15
    ATOM
                              57.084 39.761 7.907 1.00 33.09
            174 O SER 177
    ATOM
            175 N THR 178
                               58.257 38.062 8.815 1.00 25.52
    ATOM
            176 CA THR 178
                                58.508 38.772 10.064 1.00 18.93
    ATOM
                                57.828 38.064 11.258 1.00 21.81
    ATOM
            177 CB THR 178
    ATOM
            178 OG1 THR 178
                                58.348 36.736 11.394 1.00 24.18
20
            179 CG2 THR 178
                                56.330 37.971 11.032 1.00 13.81
    ATOM
                               59.993 38.967 10.358 1.00 20.69
            180 C THR 178
     ATOM
            181 O THR 178
                               60.373 39.407 11.448 1.00 20.56
     ATOM
            182 N ASN 179
                               60.837 38.645 9.385 1.00 23.68
     ATOM
                                62.275 38.802 9.555 1.00 28.22
            183 CA ASN 179
    ATOM
25
                                63.022 37.627 8.927 1.00 27.45
            184 CB ASN 179
     ATOM
                                64.460 37.529 9.402 1.00 33.98
            185 CG ASN 179
    ATOM
                                65.342 37.131 8.644 1.00 42.72
            186 OD1 ASN 179
     ATOM
            187 ND2 ASN 179
                                64.702 37.865 10.667 1.00 31.14
     ATOM
            188 C ASN 179
                               62.689 40.115 8.902 1.00 34.47
30
     ATOM
            189 O ASN 179
                               62.832 40.200 7.678 1.00 36.54
     ATOM
                               62.874 41.135 9.735 1.00 37.39
     ATOM
            190 N ALA 180
            191 CA ALA 180
                                63.235 42.479 9.292 1.00 33.71
     ATOM
                                63.555 43.352 10.494 1.00 31.57
            192 CB ALA 180
     ATOM
                               64.375 42.545 8.284 1.00 37.87
            193 C ALA 180
     ATOM
35
                               65,458 42.018 8.525 1.00 35.26
            194 O ALA 180
     ATOM
                               64.095 43.187 7.150 1.00 40.55
     ATOM
            195 N GLN 181
     ATOM
                                65.049 43.391 6.057 1.00 42.95
            196 CA GLN 181
            197 CB GLN 181
                                66,344 44.043 6.570 1.00 45.47
     ATOM
            198 CG GLN 181
                                66.144 45.326 7.383 1.00 52.70
40
     ATOM
                                65.351 46.399 6.650 1.00 55.03
            199 CD GLN 181
     ATOM
                                65.270 46.412 5.421 1.00 59.56
            200 OE1 GLN 181
     ATOM
            201 NE2 GLN 181
                                64.757 47.308 7.411 1.00 54.39
     ATOM
                               65.391 42.176 5.197 1.00 44.27
            202 C GLN 181
     ATOM
            203 O GLN 181
                               66.181 42.291 4.251 1.00 46.47
45
     ATOM
                               64.797 41.025 5.508 1.00 42.17
            204 N GLY 182
     ATOM
                                65.054 39.815 4.742 1.00 42.63
            205 CA GLY 182
     ATOM
            206 C GLY 182
207 O GLY 182
                               66.522 39.584 4.427 1.00 47.40
     ATOM
                               67.382 39.691 5.306 1.00 49.38
     ATOM
                               66.816 39.297 3.163 1.00 49.46
            208 N SER 183
50
     ATOM
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68.189 39.061 2.733 1.00 54.13
    ATOM 209 CA SER 183
                               68.208 38.225 1.449 1.00 55.08
    ATOM
           210 CB SER 183
            211 OG SER 183
                               67.197 38.647 0.546 1.00 63.54
    ATOM
                              68.949 40.369 2.532 1.00 54.84
            212 C SER 183
    ATOM
            213 O SER 183
                              70.175 40.373 2.407 1.00 56.90
    ATOM
                              68.223 41.482 2.535 1.00 55.77
           214 N HIS 184
    ATOM
                             68.854 42.775 2.342 1.00 57.78
            215 CA HIS 184
    ATOM
                             69.605 43.296 3.556 1.00 59.09
    ATOM
            216 C HIS 184
                              70.312 44.301 3.454 1.00 60.34
            217 O HIS 184
    ATOM
                              69.502 42.597 4.686 1.00 55.60
10
    ATOM
            218 N TRP 185
                               70.159 43.020 5.923 1.00 53.73
            219 CA TRP 185
    ATOM
                               69.973 41.973 7.030 1.00 50.40
    ATOM
            220 CB TRP 185
            221 CG TRP 185
                               70.746 40.694 6.837 1.00 48.09
    ATOM
            222 CD2 TRP 185
                               72.091 40.419 7.269 1.00 47.38
    ATOM
                               72.390 39.094 6.888 1.00 40.29
            223 CE2 TRP 185
    ATOM
15
                               73.071 41.169 7.937 1.00 45.43
            224 CE3 TRP 185
    ATOM
                               70.301 39.554 6.234 1.00 49.87
    ATOM
            225 CD1 TRP 185
                               71.280 38.589 6.262 1.00 48.02
            226 NE1 TRP 185
    ATOM
                               73.628 38.496 7.154 1.00 38.65
            227 CZ2 TRP 185
    ATOM
                               74.304 40.573 8.201 1.00 43.26
20
    ATOM
            228 CZ3 TRP 185
                               74.570 39.250 7.807 1.00 40.00
    ATOM
           229 CH2 TRP 185
                              71.638 43.386 5.800 1.00 55.99
    ATOM
            230 C TRP 185
    ATOM
            231 O TRP 185
                              72.089 44.359 6.401 1.00 52.84
            232 N LYS 186
                              72.389 42.614 5.021 1.00 59.15
     ATOM
                               73.818 42.863 4.843 1.00 64.01
            233 CA LYS 186
    ATOM
25
                               74.466 41.688 4.091 1.00 64.67
            234 CB LYS 186
     ATOM
                               75.943 41.868 3.729 1.00 65.58
            235 CG LYS 186
     ATOM
                               76.817 42.181 4.946 1.00 62.03
            236 CD LYS 186
     ATOM
                               78.238 42.512 4.515 1.00 61.52
            237 CE LYS 186
     ATOM
                               78.988 43.243 5.579 1.00 61.67
     ATOM
            238 NZ LYS 186
30
                              74.131 44.203 4.160 1.00 67.49
           239 C LYS 186
     ATOM
                              75.164 44.816 4.432 1.00 68.66
            240 O LYS 186
     ATOM
                               73.221 44.678 3.316 1.00 68.99
     ATOM
            241 N GLN 187
                               73.431 45.939 2.612 1.00 69.65
     ATOM 242 CA GLN 187
                                72.880 45.867 1.180 1.00 73.76
           243 CB GLN 187
     ATOM
35
                                73.632 44.935 0.237 1.00 78.61
            244 CG GLN 187
     ATOM
                                73.368 43.471 0.525 1.00 84.96
            245 CD GLN 187
     ATOM
                                74.203 42.782 1.109 1.00 87.73
            246 OE1 GLN 187
     ATOM
                                72.197 42.989 0.122 1.00 84.98
           247 NE2 GLN 187
     ATOM
                               72.817 47.141 3.323 1.00 69.16
     ATOM
           248 C GLN 187
40
                               73.379 48.235 3.299 1.00 71.39
           249 O GLN 187
     ATOM
                               71.666 46.936 3.953 1.00 65.82
     ATOM 250 N ARG 188
                                70.961 48.014 4.639 1.00 65.00
            251 CA ARG 188
     ATOM
                                69.458 47.739 4.591 1.00 66.20
            252 CB ARG 188
     ATOM
                                68.957 47.483 3.181 1.00 70.30
     ATOM 253 CG ARG 188
45
                                67.463 47.212 3.132 1.00 78.59
     ATOM
            254 CD ARG 188
                                67.003 47.008 1.760 1.00 87.71
            255 NE ARG 188
     ATOM
                                67.011 47.946 0.814 1.00 94.10
     ATOM 256 CZ ARG 188
            257 NH1 ARG 188
                                67.453 49.171 1.081 1.00 97.26
     ATOM
                                66.589 47.657 -0.409 1.00 94.07
     ATOM 258 NH2 ARG 188
50
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	ATOM	259 C ARG 188	71.409 48.286 6.077 1.00 65.39
	ATOM	260 O ARG 188	70.900 49.201 6.727 1.00 65.20
	ATOM	261 N ARG 189	72.372 47.506 6.561 1.00 64.28
	ATOM	262 CA ARG 189	72.882 47.654 7.922 1.00 60.75
5	ATOM	263 CB ARG 189	73.691 46.409 8.321 1.00 56.87
-	ATOM	264 CG ARG 189	75.050 46.308 7.630 1.00 59.52
	ATOM	265 CD ARG 189	75.580 44.891 7.589 1.00 55.86
	ATOM	266 NE ARG 189	75.874 44.348 8.907 1.00 55.48
	ATOM	267 CZ ARG 189	77.055 43.849 9.257 1.00 61.38
10	ATOM	268 NH1 ARG 189	78.057 43.832 8.388 1.00 62.54
10	ATOM	269 NH2 ARG 189	77.225 43.328 10.465 1.00 62.20
	ATOM	270 C ARG 189	73.747 48.907 8.082 1.00 60.91
	ATOM	271 O ARG 189	74.548 49.245 7.207 1.00 60.67
	ATOM	272 N LYS 190	73.575 49.591 9.207 1.00 59.06
15	ATOM	273 CA LYS 190	74.340 50.790 9.521 1.00 55.00
13	ATOM	274 CB LYS 190	73.423 52.008 9.582 1.00 55.45
	ATOM	275 C LYS 190	74.991 50.542 10.875 1.00 51.52
	ATOM	276 O LYS 190	74.320 50.144 11.830 1.00 51.68
	ATOM	277 N PHE 191	76.304 50.721 10.944 1.00 50.49
20	ATOM	278 CA PHE 191	77.037 50.508 12.186 1.00 50.17
20	ATOM	279 CB PHE 191	78.546 50.571 11.943 1.00 48.38
	ATOM	280 CG PHE 191	79.090 49.423 11.142 1.00 49.66
	ATOM	281 CD1 PHE 191	78.873 49.348 9.768 1.00 51.03
	ATOM	282 CD2 PHE 191	79.845 48.429 11.759 1.00 46.28
25	ATOM	283 CE1 PHE 191	79,403 48.298 9.018 1.00 51.35
23	ATOM	284 CE2 PHE 191	80.379 47.377 11.021 1.00 47.26
	ATOM	285 CZ PHE 191	80.158 47.311 9.646 1.00 48.48
	ATOM	286 C PHE 191	76.663 51.534 13.248 1.00 48.61
	ATOM	287 O PHE 191	76.507 52.720 12.952 1.00 50.38
30	ATOM	288 N LEU 192	76.488 51.068 14.479 1.00 47.31
50	ATOM	289 CA LEU 192	76.169 51.958 15.584 1.00 42.72
	ATOM	290 CB LEU 192	75.845 51.151 16.844 1.00 36.66
	ATOM	291 CG LEU 192	75.397 51.949 18.068 1.00 31.01
	ATOM	292 CD1 LEU 192	74.048 52.590 17.786 1.00 28.37
35	ATOM	293 CD2 LEU 192	75.318 51.043 19.289 1.00 29.60
	ATOM	294 C LEU 192	77,447 52.760 15.800 1.00 42.28
	ATOM	295 O LEU 192	78.528 52.179 15.932 1.00 39.71
	ATOM	296 N PRO 193	77.350 54.104 15.781 1.00 45.15
	ATOM	297 CD PRO 193	76.095 54.865 15.617 1.00 43.82
40	ATOM	298 CA PRO 193	78.493 55.006 15.973 1.00 43.14
. •	ATOM	299 CB PRO 193	77.820 56.306 16.400 1.00 44.37
	ATOM	300 CG PRO 193	76.571 56.308 15.565 1.00 41.66
	ATOM	301 C PRO 193	79.476 54.498 17.028 1.00 43.34
	ATOM	302 O PRO 193	79.103 54.296 18.182 1.00 45.18
45	ATOM	303 N ASP 194	80,732 54.317 16.628 1.00 44.22
	ATOM	304 CA ASP 194	81.781 53.804 17.512 1.00 47.20
	ATOM	305 CB ASP 194	83.108 53.732 16.761 1.00 41.89
	ATOM	306 C ASP 194	81.962 54.511 18.866 1.00 51.99
	ATOM	307 O ASP 194	82.636 53.986 19.752 1.00 54.04
50	ATOM	308 N ASP 195	81.381 55.698 19.025 1.00 55.21

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	ATOM	309 CA ASP 195	81.489 56.428 20.288 1.00 57.50
	ATOM	310 CB ASP 195	81.423 57.948 20.061 1.00 60.04
	ATOM	311 CG ASP 195	80.123 58.398 19.406 1.00 68.39
	ATOM	312 OD1 ASP 195	79.211 58.847 20.136 1.00 69.46
5	ATOM	313 OD2 ASP 195	80.020 58.322 18.162 1.00 72.91
	ATOM	314 C ASP 195	80.410 55.976 21.280 1.00 58.05
	ATOM	315 O ASP 195	80.540 56.180 22.491 1.00 58.97
	ATOM	316 N ILE 196	79.349 55.363 20.759 1.00 56.06
	ATOM	317 CA ILE 196	78.247 54.863 21.580 1.00 50.48
10	ATOM	318 CB ILE 196	76.930 54.762 20.766 1.00 45.82
	ATOM	319 CG2 ILE 196	75.818 54.166 21.621 1.00 44.04
	ATOM	320 CG1 ILE 196	76.517 56.147 20.261 1.00 44.27
	ATOM	321 CD1 ILE 196	75.179 56.171 19.541 1.00 45.25
	ATOM	322 C ILE 196	78.603 53.484 22.135 1.00 47.66
15	ATOM	323 O ILE 196	79.138 52.636 21.419 1.00 43.96
13	ATOM	324 N GLY 197	78.309 53.269 23.414 1.00 46.29
	ATOM	325 CA GLY 197	78.608 51.995 24.045 1.00 48.03
	ATOM	326 C GLY 197	79.978 51.963 24.692 1.00 50.42
	ATOM	327 O GLY 197	80.463 50.902 25.070 1.00 46.66
20	ATOM	328 N GLN 198	80.583 53.137 24.854 1.00 56.94
20	ATOM	329 CA GLN 198	81.910 53.259 25.454 1.00 59.51
	ATOM	330 CB GLN 198	82.751 54.257 24.649 1.00 62.53
	ATOM	331 CG GLN 198	83.232 53.718 23.316 1.00 69.39
	ATOM	331 CO GLN 198	84.088 52.484 23.483 1.00 76.76
25	ATOM	333 OE1 GLN 198	83.745 51.399 22.996 1.00 81.73
23		334 NE2 GLN 198	85.205 52.632 24.192 1.00 78.09
	ATOM ATOM	335 C GLN 198	81.915 53.678 26.922 1.00 57.56
	ATOM	336 O GLN 198	82.946 53.584 27.588 1.00 57.71
		337 N SER 199	80.770 54.128 27.425 1.00 54.11
20	ATOM	338 CA SER 199	80.676 54.600 28.800 1.00 46.28
30	ATOM	339 CB SER 199	80.243 56.067 28.777 1.00 50.28
	ATOM	340 OG SER 199	80.935 56.776 27.757 1.00 50.95
	ATOM		79.776 53.805 29.757 1.00 40.19
	ATOM		78.680 54.252 30.102 1.00 39.26
2.5	ATOM		80.236 52.629 30.214 1.00 35.63
35	ATOM	343 N PRO 200	81.530 52.011 29.904 1.00 34.88
	ATOM	344 CD PRO 200	79.464 51.789 31.139 1.00 37.54
	ATOM	345 CA PRO 200	80.223 50.457 31.124 1.00 29.86
	ATOM	346 CB PRO 200 347 CG PRO 200	81.207 50.570 29.995 1.00 34.29
40	ATOM	J., 00 1110	79.521 52.416 32.532 1.00 44.63
40	ATOM	348 C PRO 200	80.443 52.137 33.300 1.00 47.80
	ATOM	349 O PRO 200	78.532 53.241 32.867 1.00 49.57
	ATOM	350 N ILE 201	
	ATOM	351 CA ILE 201	78.525 53.924 34.158 1.00 49.15
	ATOM	352 CB ILE 201	78.213 55.426 33.990 1.00 49.19
45	ATOM	353 CG2 ILE 201	78.429 56.150 35.306 1.00 53.37
	ATOM	354 CG1 ILE 201	79.137 56.037 32.934 1.00 52.55
	ATOM	355 CD1 ILE 201	78.811 57.471 32.586 1.00 55.26
	ATOM	356 C ILE 201	77.625 53.352 35.254 1.00 49.88
_	ATOM	357 O ILE 201	78.044 53.250 36.408 1.00 50.20
50	ATOM	358 N VAL 202	76.384 53.014 34.920 1.00 47.85

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75.468 52.474 35.927 1.00 45.76
            359 CA VAL 202
    ATOM
            360 CB VAL 202
                                74.015 52.415 35.400 1.00 39.98
    ATOM
                                73.072 51.896 36.482 1.00 35.94
    ATOM
            361 CG1 VAL 202
                                73.574 53.799 34.944 1.00 29.43
    ATOM
            362 CG2 VAL 202
                               75.954 51.093 36.373 1.00 50.57
            363 C VAL 202
    ATOM
                               76.296 50.249 35.545 1.00 49.50
            364 O VAL 202
    ATOM
                               76.009 50.876 37.683 1.00 54.82
    ATOM
            365 N SER 203
                               76.490 49.609 38.223 1.00 59.26
            366 CA SER 203
    ATOM
                               77.067 49.809 39.628 1.00 64.88
            367 CB SER 203
    ATOM
                               76.127 50.428 40.492 1.00 75.47
            368 OG SER 203
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    ATOM
                               75,457 48,491 38,244 1.00 55.78
    ATOM
            369 C SER 203
                               74.285 48.712 38.544 1.00 57.50
    ATOM
            370 O SER 203
                               75.923 47.283 37.958 1.00 52.29
            371 N MET 204
    ATOM
                                75.076 46.103 37.948 1.00 50.42
            372 CA MET 204
     ATOM
            373 CB MET 204
                                75.032 45.487 36.548 1.00 47.74
    ATOM
15
                                74,243 46,297 35.541 1.00 43.40
    ATOM
            374 CG MET 204
                                72.491 46.348 35.953 1.00 40.93
            375 SD MET 204
    ATOM
                                71.947 44.785 35.241 1.00 39.19
            376 CE MET 204
    ATOM
            377 C MET 204
                               75.670 45.107 38.925 1.00 49.42
     ATOM
            378 O MET 204
                               76.892 45.020 39.062 1.00 52.25
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     ATOM
                               74.816 44.329 39.605 1.00 47.73
            379 N PRO 205
     ATOM
                                73.344 44.414 39.549 1.00 48.94
            380 CD PRO 205
     ATOM
            381 CA PRO 205
                                75.250 43.326 40.580 1.00 47.34
     ATOM
             382 CB PRO 205
                                73.982 42.513 40.810 1.00 49.44
     ATOM
                                72.907 43.562 40.725 1.00 50.62
             383 CG PRO 205
25
     ATOM
                               76.431 42.442 40.168 1.00 47.12
             384 C PRO 205
     ATOM
                               77.299 42.160 40.990 1.00 51.21
             385 O PRO 205
     ATOM
             386 N ASP 206
                               76.487 42.023 38.909 1.00 48.81
     ATOM
                                77.583 41.160 38.465 1.00 49.88
             387 CA ASP 206
     ATOM
                                77.128 40.223 37.330 1.00 54.06
             388 CB ASP 206
     ATOM
30
                                76.598 40.967 36.107 1.00 57.34
             389 CG ASP 206
     ATOM
                                77.056 42.095 35.811 1.00 52.21
     ATOM
             390 OD1 ASP 206
                                75.719 40.397 35.423 1.00 59.16
             391 OD2 ASP 206
     ATOM
                               78.902 41.843 38.093 1.00 48.70
             392 C ASP 206
     ATOM
                               79.862 41.171 37.715 1.00 49.75
             393 O ASP 206
     ATOM
35
                               78.946 43.168 38.161 1.00 47.54
             394 N GLY 207
     ATOM
                                80.174 43.869 37.820 1.00 49.23
             395 CA GLY 207
     ATOM
             396 C GLY 207
                               80.169 44.585 36.482 1.00 51.96
     ATOM
             397 O GLY 207
                               80.783 45.645 36.348 1.00 56.32
     ATOM
             398 N ASP 208
                               79.510 44.005 35.481 1.00 52.50
40
     ATOM
                                79.435 44.624 34.157 1.00 48.00
             399 CA ASP 208
     ATOM
                                78.968 43.609 33.115 1.00 53.23
     ATOM
             400 CB ASP 208
             401 CG ASP 208
                                80.038 42.592 32.774 1.00 53.17
     ATOM
                                81.130 43.006 32.335 1.00 57.42
     ATOM
             402 OD1 ASP 208
                                79.787 41.380 32.942 1.00 55.64
     ATOM
             403 OD2 ASP 208
45
                               78.497 45.823 34.187 1.00 46.68
             404 C ASP 208
     ATOM
                               77.283 45.671 34.332 1.00 45.81
             405 O ASP 208
     ATOM
                               79.075 47.014 34.077 1.00 45.95
             406 N LYS 209
     ATOM
                                78.313 48.257 34.115 1.00 45.87
             407 CA LYS 209
     ATOM
                                79.235 49.418 34.478 1.00 46.90
             408 CB LYS 209
50
     ATOM
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	ATOM	409 C LYS 209	77.561 48.546 32.812 1.00 41.17
	ATOM	410 O LYS 209	77.951 48.074 31.745 1.00 39.51
	ATOM	411 N VAL 210	76,500 49.344 32.916 1.00 39.35
	ATOM	412 CA VAL 210	75.652 49.713 31.782 1.00 38.03
5	ATOM	413 CB VAL 210	74.136 49.584 32.140 1.00 32.13
-	ATOM	414 CG1 VAL 210	73.269 49.926 30.937 1.00 27.92
	ATOM	415 CG2 VAL 210	73.818 48.183 32.627 1.00 29.43
	ATOM	416 C VAL 210	75.895 51.134 31.263 1.00 38.68
	ATOM	417 O VAL 210	76.090 52.079 32.038 1.00 39.57
10	ATOM	418 N ASP 211	75.848 51.272 29.942 1.00 39.19
	ATOM	419 CA ASP 211	76.019 52.544 29.254 1.00 38.39
	ATOM	420 CB ASP 211	76.794 52.327 27.946 1.00 40.36
	ATOM	421 CG ASP 211	77.051 53.620 27.177 1.00 36.85
	ATOM	422 OD1 ASP 211	76.193 54.528 27.167 1.00 37.95
15	ATOM	423 OD2 ASP 211	78.121 53.716 26.553 1.00 33.87
.,	ATOM	424 C ASP 211	74.601 53.040 28.958 1.00 40.60
	ATOM ·	425 O ASP 211	73.919 52.517 28.073 1.00 40.36
	ATOM	426 N LEU 212	74.185 54.074 29.680 1.00 41.55
	ATOM	427 CA LEU 212	72.854 54.664 29.552 1.00 38.39
20	ATOM	428 CB LEU 212	72.759 55.883 30.467 1.00 40.93
	ATOM	429 CG LEU 212	71.575 55.979 31.428 1.00 45.32
	ATOM	430 CD1 LEU 212	71.271 54.626 32.047 1.00 43.83
	ATOM	431 CD2 LEU 212	71.900 57.007 32.502 1.00 44.93
	ATOM	432 C LEU 212	72.448 55.050 28.133 1.00 37.61
25	ATOM	433 O LEU 212	71.318 54.805 27.719 1.00 33.71
	ATOM	434 N GLU 213	73.360 55.670 27.393 1.00 41.23
	ATOM	435 CA GLU 213	73.068 56.084 26.023 1.00 43.48
	ATOM	436 CB GLU 213	74.181 56.986 25.481 1.00 47.66
	ATOM	437 CG GLU 213	73.919 57.494 24.065 1.00 56.87
30	ATOM	438 CD GLU 213	75.121 58.180 23.433 1.00 60.87
	ATOM	439 OE1 GLU 213	76.258 57.996 23.924 1.00 60.37
	ATOM	440 OE2 GLU 213	74.921 58.894 22.423 1.00 61.13
	ATOM	441 C GLU 213	72.889 54.880 25.102 1.00 39.29
	ATOM	442 O GLU 213	71.965 54.841 24.290 1.00 36.66
35	ATOM	443 N ALA 214	73.785 53.906 25.233 1.00 36.33
	ATOM	444 CA ALA 214	73.739 52.693 24.422 1.00 34.89
	ATOM	445 CB ALA 214	74.946 51.817 24.711 1.00 30.70
	ATOM	446 C ALA 214	72.454 51.938 24.718 1.00 31.96
	ATOM	447 O ALA 214	71.739 51.523 23.804 1.00 33.93
40	ATOM	448 N PHE 215	72.151 51.798 26.003 1.00 28.47
	ATOM	449 CA PHE 215	70.947 51.116 26.445 1.00 29.74
	ATOM	450 CB PHE 215	70.819 51.223 27.962 1.00 23.73
	ATOM	451 CG PHE 215	69.589 50.568 28.515 1.00 22.71
	ATOM	452 CD1 PHE 215	69.603 49.220 28.858 1.00 22.53
45	ATOM	453 CD2 PHE 215	68.423 51.301 28.712 1.00 19.74
	ATOM	454 CE1 PHE 215	68.477 48.606 29.391 1.00 20.75
	ATOM	455 CE2 PHE 215	67.290 50.698 29.245 1.00 21.02
	ATOM	456 CZ PHE 215	67.318 49.346 29.586 1.00 19.50
	ATOM	457 C PHE 215	69.730 51.742 25.771 1.00 34.64
50	ATOM	458 O PHE 215	68.872 51.034 25.239 1.00 39.86

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	ATOM	459 N SER 216	69.677 53.071 25.771 1.00 34.78
	ATOM	460 CA SER 216	68.572 53.801 25.160 1.00 36.01
	ATOM	461 CB SER 216	68.762 55.302 25.366 1.00 37.36
	ATOM	462 OG SER 216	67.537 55.987 25.193 1.00 48.33
5	ATOM	463 C SER 216	68.458 53.475 23.664 1.00 37.06
,	ATOM	464 O SER 216	67.358 53.250 23.148 1.00 33.23
	ATOM	465 N GLU 217	69.601 53.410 22.986 1.00 36.25
		466 CA GLU 217	69.645 53.091 21.562 1.00 36.99
	ATOM		71.092 53.104 21.064 1.00 37.10
	ATOM	467 CB GLU 217	
10	ATOM	468 CG GLU 217	71.682 54.491 20.912 1.00 44.30
	ATOM	469 CD GLU 217	71.016 55.284 19.802 1.00 51.30
	ATOM	470 OE1 GLU 217	71.439 55.142 18.633 1.00 57.25
	ATOM	471 OE2 GLU 217	70.070 56.046 20.096 1.00 52.50
	ATOM	472 C GLU 217	69.019 51.726 21.286 1.00 36.93
15	ATOM	473 O GLU 217	68.191 51.577 20.381 1.00 41.06
	ATOM	474 N PHE 218	69.395 50.740 22.093 1.00 30.27
	ATOM	475 CA PHE 218	68.875 49.388 21.947 1.00 27.20
	ATOM	476 CB PHE 218	69.679 48.421 22.814 1.00 28.10
	ATOM	477 CG PHE 218	71.124 48.330 22.428 1.00 24.84
20			72.117 48.286 23.398 1.00 21.78
20	ATOM		
	ATOM	479 CD2 PHE 218	71.495 48.301 21.087 1.00 24.78
	ATOM	480 CE1 PHE 218	73.458 48.215 23.040 1.00 24.08
	ATOM	481 CE2 PHE 218	72.834 48.230 20.719 1.00 25.33
	ATOM	482 CZ PHE 218	73.818 48.187 21.697 1.00 25.04
25	ATOM	483 C PHE 218	67.381 49.281 22.261 1.00 28.23
	ATOM	484 O PHE 218	66.639 48.605 21.543 1.00 33.52
	ATOM	485 N THR 219	66.927 49.961 23.310 1.00 27.24
	ATOM	486 CA THR 219	65.515 49.913 23.666 1.00 29.28
	ATOM	487 CB THR 219	65.238 50.533 25.052 1.00 30.97
30	ATOM	488 OG1 THR 219	
50	ATOM	489 CG2 THR 219	65.901 49.712 26.149 1.00 30.78
	ATOM	490 C THR 219	64.660 50.612 22.615 1.00 33.29
	ATOM	491 O THR 219	63.473 50.317 22.474 1.00 36.85
			65.276 51.515 21.860 1.00 35.23
2.5	ATOM		64.579 52.253 20.816 1.00 38.97
35	ATOM	493 CA LYS 220	
	ATOM	494 CB LYS 220	65.506 53.334 20.236 1.00 44.67
	ATOM	495 CG LYS 220	64.805 54.491 19.513 1.00 58.02
	ATOM	496 CD LYS 220	64.406 54.130 18.079 1.00 68.57
	ATOM	497 CE LYS 220	63.732 55.296 17.347 1.00 70.50
40	ATOM	498 NZ LYS 220	62.395 55.668 17.905 1.00 66.08
	ATOM	499 C LYS 220	64.112 51.289 19.721 1.00 38.48
	ATOM	500 O LYS 220	63.021 51.446 19.173 1.00 37.18
	ATOM	501 N ILE 221	64.917 50.270 19.432 1.00 36.19
	ATOM	502 CA ILE 221	64.563 49.305 18.394 1.00 36.77
45	ATOM	503 CB ILE 221	65.756 48.996 17.457 1.00 34.41
47	ATOM	504 CG2 ILE 221	66.270 50.276 16.814 1.00 38.54
			66.864 48.267 18.221 1.00 32.93
	ATOM	505 CG1 ILE 221	
	ATOM	506 CD1 ILE 221	67.984 47.752 17.338 1.00 31.12
	ATOM	507 C ILE 221	64.002 47.971 18.888 1.00 38.22
50	ATOM	508 O ILE 221	63.499 47.181 18.089 1.00 38.90

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64.048 47.719 20.191 1.00 35.75
            509 N ILE 222
    ATOM
                               63.557 46.446 20.702 1.00 31.77
            510 CA ILE 222
    ATOM
            511 CB ILE 222
                               64.086 46.152 22.130 1.00 33.14
    ATOM
                               63.203 46.813 23.183 1.00 24.60
            512 CG2 ILE 222
    ATOM
                               64.147 44.638 22.350 1.00 32.60
            513 CG1 ILE 222
    ATOM
                               64.860 44.226 23.609 1.00 34.52
    ATOM
            514 CD1 ILE 222
                              62.042 46.240 20.624 1.00 32.56
    ATOM 515 C ILE 222
            516 O ILE 222
                              61.581 45.109 20.452 1.00 35.74
    ATOM
                               61.262 47.313 20.720 1.00 29.43
            517 N THR 223
    ATOM
                                59.806 47.170 20.651 1.00 33.57
            518 CA THR 223
10
    ATOM
                                59.075 48.514 20.903 1.00 38.99
    ATOM
            519 CB THR 223
                                59.422 49.010 22.205 1.00 41.23
    ATOM
            520 OG1 THR 223
                                57.558 48.325 20.836 1.00 36.98
    ATOM
            521 CG2 THR 223
                               59.355 46.528 19.325 1.00 31.45
            522 C THR 223
    ATOM
                               58.571 45.571 19.334 1.00 26.77
            523 O THR 223
    ATOM
15
                               59.824 47.054 18.173 1.00 31.35
    ATOM
            524 N PRO 224
                                60.570 48.306 17.950 1.00 30.11
            525 CD PRO 224
    ATOM
                                59.424 46.462 16.891 1.00 30.38
            526 CA PRO 224
    ATOM
            527 CB PRO 224
                                60.149 47.336 15.865 1.00 30.09
    ATOM
                                60.200 48.659 16.530 1.00 31.86
            528 CG PRO 224
20
    ATOM
            529 C PRO 224
                               59.882 45.007 16.795 1.00 29.51
     ATOM
            530 O PRO 224
                               59.147 44.153 16.295 1.00 32.52
    ATOM
                               61.090 44.734 17.285 1.00 22.63
            531 N ALA 225
    ATOM
            532 CA ALA 225
                                61.650 43.385 17.268 1.00 20.88
     ATOM
            533 CB ALA 225
                                63.046 43.386 17.862 1.00 20.57
25
     ATOM
                               60,752 42,416 18.026 1.00 23.53
     ATOM
            534 C ALA 225
                               60.455 41.323 17.544 1.00 25.07
            535 O ALA 225
     ATOM
     ATOM 536 N ILE 226
ATOM 537 CA ILE 226
                              60.296 42.828 19.202 1.00 22.61
                               59.420 41.989 20.007 1.00 19.46
                               59.120 42.644 21.360 1.00 20.25
            538 CB ILE 226
    ATOM
30
                               58.071 41.843 22.105 1.00 16.75
            539 CG2 ILE 226
     ATOM
                                60.401 42.772 22.182 1.00 19.30
            540 CG1 ILE 226
     ATOM
                                60.240 43.645 23.413 1.00 20.92
            541 CD1 ILE 226
     ATOM
                              58.112 41.768 19.251 1.00 21.28
     ATOM 542 C ILE 226
                              57.553 40.670 19.256 1.00 23.75
            543 O ILE 226
     ATOM
35
                               57.629 42.821 18.598 1.00 24.46
            544 N THR 227
     ATOM
                                56.393 42.752 17.826 1.00 25.81
            545 CA THR 227
     ATOM
                                56.020 44.136 17.260 1.00 31.00
            546 CB THR 227
     ATOM
                                 55,772 45,039 18,345 1.00 35,43
            547 OG1 THR 227
     ATOM
                                 54.776 44.049 16.388 1.00 29.01
            548 CG2 THR 227
40
     ATOM
                               56.508 41.728 16.691 1.00 22.85
            549 C THR 227
     ATOM
             550 O THR 227
                                55,589 40,939 16,469 1.00 22,84
     ATOM
                                57.647 41.713 16.004 1.00 16.09
            551 N ARG 228
     ATOM
                                57.862 40.765 14.919 1.00 16.97
            552 CA ARG 228
     ATOM
                                59.161 41.064 14.174 1.00 14.71
            553 CB ARG 228
45
     ATOM
                                59.137 42.369 13.391 1.00 16.22
     ATOM
            554 CG ARG 228
            555 CD ARG 228
                                60.309 42.447 12.422 1.00 20.90
     ATOM
            556 NE ARG 228
557 CZ ARG 228
                                61.595 42.207 13.078 1.00 24.94
     ATOM
                                62.243 43.113 13.805 1.00 35.06
     ATOM
                                 61.729 44.328 13.973 1.00 36.35
     ATOM
            558 NH1 ARG 228
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63.404 42.807 14.370 1.00 32.78
            559 NH2 ARG 228
    ATOM
                               57.866 39.326 15.431 1.00 21.63
            560 C ARG 228
    ATOM
                               57.477 38.407 14.704 1.00 24.47
            561 O ARG 228
    ATOM
                               58.304 39.128 16.675 1.00 20.00
            562 N VAL 229
    ATOM
                               58.319 37.793 17.266 1.00 18.39
            563 CA VAL 229
    ATOM
                               59.103 37.745 18.606 1.00 19.20
           564 CB VAL 229
    ATOM
                                58.938 36.382 19.265 1.00 14.19
           565 CG1 VAL 229
    ATOM
                                60.581 38.001 18.356 1.00 14.81
            566 CG2 VAL 229
    ATOM
           567 C VAL 229
568 O VAL 229
                               56.875 37.367 17.501 1.00 20.00
    ATOM
                               56.499 36.227 17.212 1.00 20.04
10
    ATOM
                               56.058 38.291 18.003 1.00 19.60
    ATOM
            569 N VAL 230
                                54.651 37.996 18.247 1.00 18.72
            570 CA VAL 230
    ATOM
                                53.930 39.185 18.912 1.00 22.15
            571 CB VAL 230
    ATOM
                                52.452 38.862 19.113 1.00 15.66
            572 CG1 VAL 230
     ATOM
            573 CG2 VAL 230
                                54.592 39.522 20.248 1.00 21.05
    ATOM
15
                               53.967 37.660 16.917 1.00 26.17
    ATOM 574 C VAL 230
                               53.188 36.704 16.836 1.00 28.01
            575 O VAL 230
    ATOM
                               54.288 38.426 15.873 1.00 25.07
           576 N ASP 231
     ATOM
                               53.714 38.216 14.542 1.00 26.10
     ATOM 577 CA ASP 231
                               54.169 39.309 13.568 1.00 22.15
     ATOM 578 CB ASP 231
20
            579 CG ASP 231
                               53.620 40.684 13.921 1.00 29.49
     ATOM
                                52.587 40.767 14.624 1.00 30.93
     ATOM
            580 OD1 ASP 231
                                54.223 41.687 13.481 1.00 31.74
            581 OD2 ASP 231
     ATOM
                              54.087 36.842 13.989 1.00 27.35
            582 C ASP 231
     ATOM
                               53.245 36.154 13.408 1.00 25.89
            583 O ASP 231
25
     ATOM
                               55.347 36.451 14.175 1.00 24.29
            584 N PHE 232
     ATOM
                                55.825 35.154 13.714 1.00 22.90
            585 CA PHE 232
     ATOM
            586 CB PHE 232
                                57.302 34.956 14.090 1.00 20.56
     ATOM
                                57.762 33.525 14.007 1.00 24.20
     ATOM 587 CG PHE 232
                                57.952 32.910 12.772 1.00 23.44
            588 CD1 PHE 232
     ATOM
30
                                57.959 32.776 15.167 1.00 19.41
            589 CD2 PHE 232
     ATOM
                                58.329 31.567 12.689 1.00 19.53
     ATOM 590 CE1 PHE 232
                               58.336 31.431 15.100 1.00 21.09
     ATOM 591 CE2 PHE 232
                               58.520 30.824 13.858 1.00 21.61
            592 CZ PHE 232
     ATOM
                               54.984 34.047 14.341 1.00 24.18
            593 C PHE 232
     ATOM
35
                               54.481 33.160 13.645 1.00 22.26
            594 O PHE 232
     ATOM
                               54.810 34.127 15.656 1.00 23.90
            595 N ALA 233
     ATOM
                                54.048 33.128 16.397 1.00 22.60
            596 CA ALA 233
     ATOM
                                54.088 33.435 17.890 1.00 15.34
     ATOM
            597 CB ALA 233
                               52.609 33.040 15.917 1.00 22.04
            598 C ALA 233
40
     ATOM
                               52.084 31.948 15.697 1.00 22.86
             599 O ALA 233
     ATOM
                               51.978 34.195 15.743 1.00 25.04
            600 N LYS 234
     ATOM
                                50.593 34.248 15.298 1.00 27.68
            601 CA LYS 234
     ATOM
                                50.096 35.691 15.292 1.00 31.41
     ATOM
            602 CB LYS 234
                                49.845 36.248 16.682 1.00 40.37
            603 CG LYS 234
     ATOM
45
                                49.212 37.626 16.604 1.00 57.53
     ATOM 604 CD LYS 234
                                48.772 38.112 17.974 1.00 64.28
            605 CE LYS 234
     ATOM
                                48.164 39.473 17.904 1.00 67.19
            606 NZ LYS 234
     ATOM
                               50.358 33.588 13.939 1.00 26.42
            607 C LYS 234
     ATOM
                               49.269 33.067 13.674 1.00 31.34
            608 O LYS 234
     ATOM
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ATOM 610 CA LYS 235 51.278 32.985 11.770 1.00 26.4 ATOM 611 CB LYS 235 52.244 33.664 10.805 1.00 24.9 ATOM 612 CG LYS 235 52.244 33.664 10.805 1.00 24.9 ATOM 613 CD LYS 235 52.843 35.775 9.588 1.00 29.3 ATOM 614 CE LYS 235 52.843 35.775 9.588 1.00 29.3 ATOM 615 NZ LYS 235 53.354 37.869 8.376 1.00 40.1 ATOM 616 C LYS 235 53.354 37.869 8.376 1.00 40.1 ATOM 617 O LYS 235 51.470 31.469 11.759 1.00 30.33 ATOM 618 N LEU 236 51.470 31.469 11.759 1.00 30.33 ATOM 619 CA LEU 236 51.722 30.889 12.930 1.00 32.39 ATOM 620 CB LEU 236 52.944 29.080 14.089 1.00 29.9 ATOM 621 CG LEU 236 54.373 29.516 13.765 1.00 24.6 ATOM 622 CD1 LEU 236 55.299 29.054 14.877 1.00 22. ATOM 623 CD2 LEU 236 55.299 29.054 14.877 1.00 24.6 ATOM 624 C LEU 236 50.520 28.891 13.470 1.00 41.4 ATOM 625 O LEU 236 50.520 28.891 13.470 1.00 41.4 ATOM 626 N PRO 237 50.012 27.895 12.729 1.00 47.8 ATOM 627 CD PRO 237 50.012 27.895 12.729 1.00 47.8 ATOM 629 CB PRO 237 48.669 26.128 11.962 1.00 55.2 ATOM 630 CG PRO 237 48.669 26.128 11.962 1.00 55.2 ATOM 631 C PRO 237 48.669 26.128 11.962 1.00 55.2 ATOM 630 CG PRO 237 48.669 26.128 11.962 1.00 55.2 ATOM 631 C PRO 237 47.533 27.134 15.087 1.00 42.4 ATOM 630 CG PRO 237 47.533 27.134 15.087 1.00 42.5 ATOM 633 N MET 238 49.315 25.927 14.906 1.00 49.5 ATOM 636 CG MET 238 50.379 24.275 16.424 1.00 52. ATOM 638 CE MET 238 50.379 24.275 16.424 1.00 52. ATOM 639 C MET 238 49.306 25.354 16.245 1.00 54.0 ATOM 630 C MET 238 49.352 26.362 17.395 1.00 54.0 ATOM 640 O MET 238 49.352 26.362 17.395 1.00 54.0 ATOM 641 N PHE 239 49.803 27.578 17.101 1.00 50.1	LYS 235 51.278 32.985 11.770 1.00 26.42 LYS 235 52.244 33.664 10.805 1.00 24.92 LYS 235 51.908 35.127 10.583 1.00 22.41 LYS 235 52.843 35.775 9.588 1.00 29.38 LYS 235 52.481 37.234 9.395 1.00 33.49 LYS 235 51.470 31.469 11.759 1.00 30.02 LYS 235 51.417 30.838 10.699 1.00 30.37 LEU 236 51.722 30.889 12.930 1.00 32.39 LEU 236 51.878 29.443 13.053 1.00 36.24 3 LEU 236 52.944 29.080 14.089 1.00 29.91 3 LEU 236 52.944 29.080 14.089 1.00 29.91 3 LEU 236 52.944 29.080 14.089 1.00 29.91 54.811 28.942 12.427 1.00 24.48 50 2 LEU 236 55.299 29.054 14.877 1.00 22.71 54.811 28.942 12.427 1.00 24.48 50 PRO 237 50.012 27.895 12.729 1.00 44.86 50 PRO 237 50.012 27.895 12.729 1.00 47.86 50 PRO 237 48.713 27.262 12.992 1.00 50.28 50 PRO 237 48.669 26.128 11.962 1.00 55.25 50 PRO 237 48.495 26.751 14.422 1.00 47.94 49.306 25.354 16.245 1.00 53.49 50 MET 238 50.379 24.275 16.424 1.00 50.16 50 MET 238 <		ATOM	609 N LYS 235	51.382 33.588 13.093 1.00 24.38
ATOM 611 CB LYS 235 52.244 33.664 10.805 1.00 24.9 ATOM 612 CG LYS 235 51.908 35.127 10.583 1.00 22.4 5 ATOM 613 CD LYS 235 52.843 35.775 9.588 1.00 29.3 ATOM 614 CE LYS 235 52.843 35.775 9.588 1.00 29.3 ATOM 615 NZ LYS 235 53.354 37.869 8.376 1.00 40.13 ATOM 616 C LYS 235 53.354 37.869 8.376 1.00 40.13 ATOM 617 O LYS 235 51.470 31.469 11.759 1.00 30.02 ATOM 618 N LEU 236 51.472 30.889 12.930 1.00 32.39 ATOM 619 CA LEU 236 51.878 29.443 13.053 1.00 36.2 ATOM 620 CB LEU 236 52.944 29.080 14.089 1.00 29.9 ATOM 621 CG LEU 236 54.373 29.516 13.765 1.00 24.6 ATOM 622 CD1 LEU 236 55.299 29.054 14.877 1.00 22. 15 ATOM 623 CD2 LEU 236 54.373 29.516 13.765 1.00 24.6 ATOM 624 C LEU 236 50.520 28.891 13.470 1.00 41.2 ATOM 625 O LEU 236 50.520 28.891 13.470 1.00 41.2 ATOM 626 N PRO 237 50.012 27.895 12.729 1.00 47.8 ATOM 627 CD PRO 237 50.012 27.895 12.729 1.00 49.3 ATOM 628 CA PRO 237 48.669 26.128 11.962 1.00 55.2 ATOM 630 CG PRO 237 47.533 27.134 15.087 1.00 49.4 25 ATOM 631 C PRO 237 47.533 27.134 15.087 1.00 49.5 ATOM 632 O PRO 237 47.533 27.134 15.087 1.00 49.5 ATOM 635 CB MET 238 49.415 25.927 14.906 1.00 49.5 ATOM 636 CG MET 238 50.028 22.959 15.728 1.00 56. ATOM 637 SD MET 238 50.028 22.959 15.728 1.00 56. ATOM 638 CE MET 238 50.896 21.440 13.552 1.00 55. ATOM 639 C MET 238 49.352 26.362 17.395 1.00 54.2 ATOM 640 O MET 238 48.930 26.058 18.515 1.00 54.2 ATOM 641 N PHE 239 49.803 27.578 17.101 1.00 50.1	6 LYS 235 52.244 33.664 10.805 1.00 24.92 6 LYS 235 51.908 35.127 10.583 1.00 22.41 6 LYS 235 52.843 35.775 9.588 1.00 29.38 6 LYS 235 52.481 37.234 9.395 1.00 30.34 6 LYS 235 51.470 31.469 11.759 1.00 30.02 6 LYS 235 51.417 30.838 10.699 1.00 30.37 6 LEU 236 51.722 30.889 12.930 1.00 30.37 6 LEU 236 51.878 29.443 13.053 1.00 30.37 7 LEU 236 52.944 29.080 14.089 1.00 29.91 6 LEU 236 52.994 29.080 14.089 1.00 22.71 5 LEU 236 52.999 29.054 14.877 1.00 22.71 5 LEU 236 52.999 29.054 14.877 1.00 24.48 6 LEU 236 50.520 2				
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	51.336 30.607 18.826 1.00 30.25 51.336 30.607 18.826 1.00 30.25 52.127 30.332 19.937 1.00 25.66 52.127 30.332 19.937 1.00 25.66 52.127 30.332 19.937 1.00 25.66 52.128 31.307 20.896 1.00 30.28 52.249 51.019 32.862 19.644 1.00 30.49 51.813 32.576 20.750 1.00 29.00 62.249 PHE 239 48.647 29.434 18.337 1.00 35.65 63.240 PHE 239 48.151 29.521 19.457 1.00 30.27 64.250 SER 240 46.936 30.866 17.359 1.00 36.49 64.251 A SER 240 46.936 30.866 17.359 1.00 36.37	35			
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	E2 PHE 239 51.019 32.862 19.644 1.00 30.49 Z PHE 239 51.813 32.576 20.750 1.00 29.00 PHE 239 48.647 29.434 18.337 1.00 35.65 PHE 239 48.151 29.521 19.457 1.00 30.27 SER 240 48.133 30.037 17.272 1.00 36.49 A SER 240 46.936 30.866 17.359 1.00 36.37				52.368 31.307 20.896 1.00 30.28
	Z PHE 239 51.813 32.576 20.750 1.00 29.00 PHE 239 48.647 29.434 18.337 1.00 35.65 PHE 239 48.151 29.521 19.457 1.00 30.27 SER 240 48.133 30.037 17.272 1.00 36.49 A SER 240 46.936 30.866 17.359 1.00 36.37	40	_		
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	PHE 239 48.151 29.521 19.457 1.00 30.27 SER 240 48.133 30.037 17.272 1.00 36.49 A SER 240 46.936 30.866 17.359 1.00 36.37				
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		45			
	3 SER 240 40.022 51.400 15.55 1.400 50.05	-			46.622 31.466 15.994 1.00 35.87
ATOM 655 C SER 240 45.707 30.145 17.936 1.00 40.3	SER 240 45.707 30.145 17.936 1.00 40.37				
	SER 240 44.784 30.789 18.438 1.00 37.47		ATOM		44.784 30.789 18.438 1.00 37.47
			ATOM	657 N GLU 241	45.713 28.814 17.889 1.00 43.00
ATOM 657 N GLU 241 45.713 28.814 17.889 1.00 43.0		50	ATOM	658 CA GLU 241	44.605 28.004 18.404 1.00 46.31
	OTTI 241 45 712 20 014 17 000 1 00 42 00				
ATOM 657 N GLU 241 45.713 28.814 17.889 1.00 43.0		50	ATUM	658 CA GLU 241	44.003 28.004 18.404 1.00 46.31

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	ATOM	659 CB GLU 241	44.714 26.566 17.881 1.00 55.84
	ATOM	660 CG GLU 241	44.750 26.422 16.360 1.00 69.03
	ATOM	661 CD GLU 241	45.141 25.015 15.900 1.00 74.99
_	ATOM	662 OE1 GLU 241	45.835 24.299 16.658 1.00 77.81
5	ATOM	663 OE2 GLU 241	44.765 24.629 14.770 1.00 70.58
	ATOM	664 C GLU 241	44.587 27.961 19.933 1.00 42.60
	ATOM	665 O GLU 241	43.541 27.740 20.545 1.00 43.23
	ATOM	666 N LEU 242	45.762 28.125 20.535 1.00 39.31
	ATOM	667 CA LEU 242	45.926 28.086 21.987 1.00 34.54
10	ATOM	668 CB LEU 242	47.417 28.109 22.344 1.00 28.35
	ATOM	669 CG LEU 242	48.311 26.974 21.853 1.00 27.59
	ATOM	670 CD1 LEU 242	49.750 27.307 22.180 1.00 20.72
	ATOM	671 CD2 LEU 242	47.902 25.661 22.500 1.00 24.97
	ATOM	672 C LEU 242	45.242 29.240 22.711 1.00 32.23
15	ATOM	673 O LEU 242	44,956 30.282 22.119 1.00 31.50
	ATOM	674 N PRO 243	44.954 29.060 24.010 1.00 34.39
	ATOM	675 CD PRO 243	45.118 27.843 24.827 1.00 31.68
	ATOM	676 CA PRO 243	44.309 30.134 24.773 1.00 34.39
	ATOM	677 CB PRO 243	44.092 29.498 26.154 1.00 32.34
20	ATOM	678 CG PRO 243	44.081 28.026 25.892 1.00 33.80
	ATOM	679 C PRO 243	45.300 31.303 24.873 1.00 35.56
	ATOM	680 O PRO 243	46.517 31.082 24.897 1.00 34.99
	ATOM	681 N CYS 244	44.791 32.532 24.946 1.00 34.23
	ATOM	682 CA CYS 244	45.648 33.714 25.062 1.00 37.03
25	ATOM	683 CB CYS 244	44.820 34.960 25.376 1.00 43.49
	ATOM	684 SG CYS 244	43.820 35.531 24.007 1.00 71.28
	ATOM	685 C CYS 244	46.716 33.555 26.135 1.00 34.99
	ATOM	686 O CYS 244	47.894 33.802 25.882 1.00 37.49
	ATOM	687 N GLU 245	46.305 33.125 27.326 1.00 33.03
30	ATOM	688 CA GLU 245	47.249 32.944 28.424 1.00 35.72
50	ATOM	689 CB GLU 245	46.559 32.469 29.716 1.00 37.85
	ATOM	690 CG GLU 245	45.294 31.633 29.549 1.00 46.81
	ATOM	691 CD GLU 245	44.029 32.478 29.480 1.00 44.81
	ATOM	692 OE1 GLU 245	43,606 33.012 30.527 1.00 33.05
35	ATOM	693 OE2 GLU 245	43.454 32.599 28.377 1.00 48.22
55	ATOM	694 C GLU 245	48.414 32.035 28.047 1.00 32.29
	ATOM	695 O GLU 245	49.558 32.319 28.399 1.00 35.92
	ATOM	696 N ASP 246	48.134 30.975 27.295 1.00 30.64
	ATOM	697 CA ASP 246	49.182 30.058 26.855 1.00 28.23
40			
40	ATOM	698 CB ASP 246	48.575 28.809 26.208 1.00 30.51 48.213 27.737 27.222 1.00 33.18
	ATOM	699 CG ASP 246	48.265 28.006 28.439 1.00 31.26
	ATOM	700 OD1 ASP 246	
	ATOM	701 OD2 ASP 246	47.884 26.613 26.796 1.00 33.85
4.5	ATOM	702 C ASP 246	50.104 30.757 25.860 1.00 30.10
45	ATOM	703 O ASP 246	51.330 30.651 25.950 1.00 27.08
	ATOM	704 N GLN 247	49.500 31.477 24.918 1.00 30.39
	ATOM	705 CA GLN 247	50.249 32.208 23.901 1.00 29.08
	ATOM	706 CB GLN 247	49.295 32.949 22.964 1.00 27.34
	ATOM	707 CG GLN 247	48.390 32.034 22.147 1.00 28.95
50	ATOM	708 CD GLN 247	47.531 32.796 21.153 1.00 30.74

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47.850 33.918 20.767 1.00 33.23
     ATOM
             709 OE1 GLN 247
                                 46.439 32.185 20.729 1.00 35.19
             710 NE2 GLN 247
     ATOM
                                51.190 33.196 24.575 1.00 27.51
             711 C GLN 247
     ATOM
                                52.377 33.261 24.256 1.00 28.70
     ATOM
            712 O GLN 247
                               50.661 33.921 25.552 1.00 27.81
    ATOM
            713 N ILE 248
                               51.431 34.908 26.295 1.00 29.41
     ATOM
            714 CA ILE 248
     ATOM
            715 CB ILE 248
                               50.525 35.662 27.303 1.00 28.96
                                51.356 36.476 28.279 1.00 28.67
            716 CG2 ILE 248
     ATOM
                                49.555 36.571 26.543 1.00 28.83
            717 CG1 ILE 248
     ATOM
            718 CD1 ILE 248
                                48.514 37.236 27.420 1.00 30.76
10
     ATOM
                              52.618 34.259 27.006 1.00 28.39
            719 C ILE 248
     ATOM
                              53.759 34.715 26.869 1.00 27.88
    ATOM
            720 O ILE 248
                              52.356 33.177 27.732 1.00 26.07
            721 N ILE 249
    ATOM
            722 CA ILE 249
                               53.413 32.474 28.454 1.00 27.37
     ATOM
            723 CB ILE 249
                               52.839 31.294 29.281 1.00 30.32
15
     ATOM
            724 CG2 ILE 249
                                53.958 30.425 29.840 1.00 31.29
     ATOM
                                51.987 31.831 30.429 1.00 30.31
     ATOM
            725 CG1 ILE 249
                                51.295 30.753 31.230 1.00 31.30
     ATOM
            726 CD1 ILE 249
     ATOM
            727 C ILE 249
                              54.510 31.974 27.509 1.00 28.63
20
     ATOM
            728 O ILE 249
                              55.701 32.100 27.808 1.00 29.59
            729 N LEU 250
                               54.110 31.442 26.357 1.00 29.03
     ATOM
            730 CA LEU 250
                                55.068 30.934 25.380 1.00 22.44
     ATOM
                                54.351 30.166 24.266 1.00 24.30
            731 CB LEU 250
     ATOM
                                53.665 28.866 24.687 1.00 23.20
            732 CG LEU 250
     ATOM
            733 CD1 LEU 250
                                 52.951 28.273 23.502 1.00 20.36
     ATOM
25
                                 54.685 27.880 25.238 1.00 19.45
     ATOM
            734 CD2 LEU 250
                               55.919 32.055 24.794 1.00 18.97
     ATOM
             735 C LEU 250
             736 O LEU 250
                               57.133 31.903 24.648 1.00 18.37
     ATOM
            737 N LEU 251
                                55.291 33.180 24.468 1.00 20.63
     ATOM
            738 CA LEU 251
                                56.026 34.318 23.915 1.00 27.43
30
     ATOM
            739 CB LEU 251
                                55.065 35.412 23.449 1.00 22.92
     ATOM
                                54.364 35.093 22.128 1.00 24.72
            740 CG LEU 251
     ATOM
                                 53.342 36.167 21.821 1.00 32.13
            741 CD1 LEU 251
     ATOM
                                 55.389 34.981 21.009 1.00 22.46
            742 CD2 LEU 251
     ATOM
                               57.026 34.875 24.930 1.00 27.23
            743 C LEU 251
35
     ATOM
                                58.202 35.078 24.614 1.00 26.48
            744 O LEU 251
     ATOM
                               56.561 35.094 26.156 1.00 27.34
            745 N LYS 252
     ATOM
                                57.425 35.598 27.215 1.00 28.95
            746 CA LYS 252
     ATOM
                                56.649 35.715 28.527 1.00 32.89
            747 CB LYS 252
     ATOM
            748 CG LYS 252
                                55.570 36.783 28.530 1.00 35.06
40
     ATOM
             749 CD LYS 252
                                55.084 37.028 29.943 1.00 42.82
     ATOM
                                54.124 38.191 30.003 1.00 53.05
            750 CE LYS 252
     ATOM
                                53.677 38.451 31.398 1.00 64.03
     ATOM
            751 NZ LYS 252
                               58.605 34.647 27.405 1.00 27.66
            752 C LYS 252
     ATOM
                                59.734 35.076 27.646 1.00 33.16
            753 O LYS 252
45
     ATOM
            754 N GLY 253
                                58.344 33.357 27.243 1.00 24.50
     ATOM
            755 CA GLY 253
                                59.386 32.364 27.402 1.00 22.33
     ATOM
            756 C GLY 253
757 O GLY 253
                                60.423 32.273 26.297 1.00 23.99
     ATOM
                                61.589 32.016 26.581 1.00 30.77
     ATOM
                                60.041 32.526 25.049 1.00 22.66
50
     ATOM
            758 N CYS 254
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	ATOM	759 CA CYS 254	60.986 32.405 23.934 1.00 20.75
	ATOM	760 CB CYS 254	60.386 31.494 22.868 1.00 24.86
	ATOM	761 SG CYS 254	58.996 32.276 22.014 1.00 25.55
	ATOM	762 C CYS 254	61.399 33.702 23.242 1.00 23.79
5	ATOM	763 O CYS 254	62.262 33.685 22.357 1.00 22.18
	ATOM	764 N CYS 255	60.788 34.814 23.625 1.00 19.49
	ATOM	765 CA CYS 255	61.084 36.085 22.981 1.00 21.08
	ATOM	766 CB CYS 255	60.336 37.220 23.669 1.00 18.21
	ATOM	767 SG CYS 255	60.264 38.713 22.677 1.00 22.96
10	ATOM	768 C CYS 255	62.570 36.413 22.842 1.00 21.87
	ATOM	769 O CYS 255	63.050 36.641 21.729 1.00 22.23
	ATOM	770 N MET 256	63,310 36,397 23,947 1.00 20.82
	ATOM	771 CA MET 256	64.741 36.706 23.895 1.00 20.50
	ATOM	772 CB MET 256	65.322 36.801 25.312 1.00 22.50
15	ATOM	773 CG MET 256	66.808 37.139 25.354 1.00 16.67
	ATOM	774 SD MET 256	67.205 38.732 24.605 1.00 24.46
	ATOM	775 CE MET 256	69.027 38.764 24.791 1.00 19.21
	ATOM	776 C MET 256	65.510 35.667 23.072 1.00 18.38
	ATOM	777 O MET 256	66.401 36.005 22.293 1.00 17.68
20	ATOM	778 N GLU 257	65.149 34.404 23.248 1.00 20.33
	ATOM	779 CA GLU 257	65.779 33.308 22.526 1.00 21.08
	ATOM	780 CB GLU 257	65.148 31.982 22.943 1.00 22.28
	ATOM	781 CG GLU 257	65,374 31.640 24.411 1.00 34.68
	ATOM	782 CD GLU 257	64.515 30.486 24.907 1.00 43.20
25	ATOM	783 OE1 GLU 257	
	ATOM	784 OE2 GLU 257	
	ATOM	785 C GLU 257	65.650 33.503 21.018 1.00 19.26
	ATOM	786 O GLU 257	66.632 33.360 20.276 1.00 18.09
	ATOM	787 N ILE 258	64.446 33.850 20.566 1.00 16.30
30	ATOM	788 CA ILE 258	64.199 34.065 19.141 1.00 18.09
	ATOM	789 CB ILE 258	62.677 34.150 18.825 1.00 18.61
	ATOM	790 CG2 ILE 258	62.441 34.653 17.395 1.00 16.23
	ATOM	791 CG1 ILE 258	62.032 32.771 19.021 1.00 13.80
	ATOM	792 CD1 ILE 258	60.544 32.714 18.695 1.00 13.21
35	ATOM	793 C ILE 258	64.948 35.297 18.638 1.00 20.12
	ATOM	794 O ILE 258	65.605 35.242 17.593 1.00 19.17
	ATOM	795 N MET 259	
	ATOM	796 CA MET 259	
	ATOM	797 CB MET 259	65.249 38.772 19.941 1.00 18.80
40	ATOM	798 CG MET 259	63.782 39.159 19.894 1.00 17.66
. •	ATOM	799 SD MET 259	63.457 40.748 20.678 1.00 25.77
	ATOM	800 CE MET 259	63.774 40.377 22.374 1.00 16.65
	ATOM	801 C MET 259	67.111 37.397 18.973 1.00 19.51
	ATOM	802 O MET 259	67.797 37.913 18.080 1.00 25.53
45	ATOM	803 N SER 260	67.625 36.605 19.908 1.00 19.58
.,	ATOM	804 CA SER 260	69.056 36.324 19.947 1.00 16.90
	ATOM	805 CB SER 260	69.434 35.631 21.251 1.00 15.56
	ATOM	806 OG SER 260	69.093 36.455 22.352 1.00 22.98
	ATOM	807 C SER 260	69.471 35.487 18.746 1.00 14.52
50	ATOM	808 O SER 260	70.496 35.761 18.129 1.00 22.82

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	ATOM	809 N LEU 261	68.663 34.490 18.397 1.00 16.50
	ATOM	810 CA LEU 261	68.948 33.642 17.241 1.00 17.78
	ATOM	811 CB LEU 261	67.878 32.552 17.092 1.00 18.38
	ATOM	812 CG LEU 261	67.890 31.708 15.812 1.00 14.47
5	ATOM	813 CD1 LEU 261	69.159 30.877 15.728 1.00 16.76
	ATOM	814 CD2 LEU 261	66.672 30.806 15.793 1.00 14.06
	ATOM	815 C LEU 261	68.959 34.519 15.992 1.00 20.40
	ATOM	816 O LEU 261	69.885 34.450 15.181 1.00 22.00
	ATOM	817 N ARG 262	67.934 35.356 15.854 1.00 21.02
10	ATOM	818 CA ARG 262	67.821 36.249 14.705 1.00 22.84
	ATOM	819 CB ARG 262	66.530 37.067 14.782 1.00 20.29
	ATOM	820 CG ARG 262	65.311 36.267 14.364 1.00 23.33
	ATOM	821 CD ARG 262	64.007 37.026 14.509 1.00 19.05
	ATOM	822 NE ARG 262	62.959 36.321 13.775 1.00 21.32
15	ATOM	823 CZ ARG 262	61.780 36.837 13.441 1.00 23.44
10	ATOM	824 NH1 ARG 262	61.465 38.081 13.780 1.00 22.99
	ATOM	825 NH2 ARG 262	60.933 36.116 12.713 1.00 22.09
	ATOM	826 C ARG 262	69.035 37.154 14.561 1.00 22.66
	ATOM	827 O ARG 262	69.434 37.483 13.445 1.00 22.41
20	ATOM	828 N ALA 263	69.625 37.545 15.689 1.00 23.52
20	ATOM	829 CA ALA 263	70.820 38.386 15.677 1.00 22.37
	ATOM	830 CB ALA 263	70.986 39.089 17.018 1.00 22.76
	ATOM	831 C ALA 263	72.052 37.530 15.366 1.00 22.85
	ATOM	832 O ALA 263	72.882 37.897 14.529 1.00 25.50
25	ATOM	833 N ALA 264	72.131 36.365 16.005 1.00 21.68
2,	ATOM	834 CA ALA 264	73.242 35.438 15.826 1.00 20.26
	ATOM	835 CB ALA 264	73.092 34.256 16.763 1.00 15.97
	ATOM	836 C ALA 264	73.401 34.957 14.382 1.00 23.11
	ATOM	837 O ALA 264	74.523 34.831 13.892 1.00 24.87
30	ATOM	838 N VAL 265	72.293 34.679 13.697 1.00 22.94
50	ATOM	839 CA VAL 265	72.380 34.226 12.306 1.00 28.98
	ATOM	840 CB VAL 265	71.072 33.547 11.797 1.00 25.97
	ATOM	841 CG1 VAL 265	70.751 32.330 12.638 1.00 26.27
	ATOM	842 CG2 VAL 265	69.907 34.527 11.797 1.00 26.64
35	ATOM	843 C VAL 265	72.761 35.373 11.369 1.00 28.81
33	ATOM	844 O VAL 265	72.966 35.160 10.176 1.00 31.92
	ATOM	845 N ARG 266	72.830 36.587 11.915 1.00 31.83
	ATOM	846 CA ARG 266	73.210 37.774 11.150 1.00 33.19
	ATOM	847 CB ARG 266	72.141 38.861 11.258 1.00 31.67
40	ATOM	848 CG ARG 266	70.986 38.623 10.320 1.00 26.82
40	ATOM	849 CD ARG 266	69.913 39.668 10.454 1.00 33.95
	ATOM	850 NE ARG 266	68.955 39.532 9.361 1.00 38.15
	ATOM	851 CZ ARG 266	67.688 39.927 9.410 1.00 37.39
			67.198 40.491 10.509 1.00 29.92
15	ATOM ATOM		66.918 39.770 8.340 1.00 31.24
45			74.565 38.307 11.604 1.00 36.31
	ATOM	854 C ARG 266 855 O ARG 266	74.821 39.516 11.575 1.00 38.56
	ATOM		75.416 37.393 12.056 1.00 34.21
	ATOM	856 N TYR 267	75.416 37.393 12.036 1.00 34.21 76.755 37.733 12.502 1.00 35.24
50	ATOM	857 CA TYR 267	77.283 36.640 13.440 1.00 32.37
50	ATOM	858 CB TYR 267	11.283 30.040 13.440 1.00 32.37

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78.774 36.699 13.703 1.00 35.07
            859 CG TYR 267
    ATOM
            860 CD1 TYR 267
                                79.303 37.555 14.669 1.00 33.94
    ATOM
            861 CE1 TYR 267
                                80.677 37.609 14.905 1.00 36.60
    ATOM
                                79.658 35.894 12.979 1.00 34.68
            862 CD2 TYR 267
    ATOM
                                81.029 35.940 13.208 1.00 36.07
            863 CE2 TYR 267
    ATOM
                                81.533 36.797 14.170 1.00 37.14
            864 CZ TYR 267
    ATOM
                                82.889 36.835 14.396 1.00 41.52
            865 OH TYR 267
    ATOM
            866 C TYR 267
                               77.639 37.831 11.263 1.00 37.68
    ATOM
                               77.609 36.943 10.410 1.00 36.48
            867 O TYR 267
    ATOM
                               78,400 38,915 11.150 1.00 39.58
            868 N ASP 268
10
    ATOM
                               79.301 39.096 10.016 1.00 42.77
            869 CA ASP 268
    ATOM
                               79.170 40.511 9.434 1.00 44.38
            870 CB ASP 268
    ATOM
                                80.145 40.770 8.290 1.00 50.31
            871 CG ASP 268
    ATOM
            872 OD1 ASP 268
                                80.290 39.901 7.400 1.00 55.79
     ATOM
            873 OD2 ASP 268
                                80.773 41.847 8.280 1.00 50.24
     ATOM
15
                               80,737 38.846 10.466 1.00 42.51
     ATOM
            874 C ASP 268
                               81.305 39.645 11.208 1.00 42.75
    ATOM
            875 O ASP 268
                               81.346 37.733 10.020 1.00 44.56
            876 N PRO 269
     ATOM
                                80.770 36.697 9.146 1.00 42.66
            877 CD PRO 269
     ATOM
            878 CA PRO 269
                                82.725 37.395 10.393 1.00 45.98
20
     ATOM
                                82.991 36.111 9.607 1.00 44.04
            879 CB PRO 269
     ATOM
                                81.631 35.506 9.458 1.00 43.33
            880 CG PRO 269
     ATOM
                               83.710 38.492 10.004 1.00 50.31
     ATOM
            881 C PRO 269
                               84.630 38.800 10.761 1.00 49.83
            882 O PRO 269
     ATOM
                               83.486 39.100 8.840 1.00 53.62
             883 N ALA 270
25
     ATOM
                                84.348 40.165 8.329 1.00 54.54
             884 CA ALA 270
     ATOM
                                83.892 40.585 6.929 1.00 51.24
     ATOM
             885 CB ALA 270
                               84,449 41.389 9.248 1.00 55.69
             886 C ALA 270
     ATOM
             887 O ALA 270
                               85.488 42.045 9.294 1.00 57.92
     ATOM
             888 N SER 271
                               83.384 41.685 9.989 1.00 54.71
     ATOM
30
             889 CA SER 271
                                83.378 42.838 10.889 1.00 51.26
     ATOM
                                82.182 43.740 10.575 1.00 49.92
             890 CB SER 271
     ATOM
                                82.065 43.976 9.183 1.00 60.09
             891 OG SER 271
     ATOM
                               83.305 42.443 12.360 1.00 50.78
             892 C SER 271
     ATOM
                               83.482 43.288 13.240 1.00 52.11
             893 O SER 271
35
     ATOM
                               83.051 41.162 12.619 1.00 48.96
             894 N ASP 272
     ATOM
                                82.898 40.643 13.978 1.00 45.53
             895 CA ASP 272
     ATOM
                                84.206 40.765 14.776 1.00 44.82
             896 CB ASP 272
     ATOM
                                84.142 40.064 16.131 1.00 47.66
             897 CG ASP 272
     ATOM
                                84.750 40.581 17.091 1.00 48.64
             898 OD1 ASP 272
40
     ATOM
             899 OD2 ASP 272
                                 83.495 38.999 16.238 1.00 43.85
     ATOM
                               81.765 41.437 14.636 1.00 44.46
             900 C ASP 272
     ATOM
             901 O ASP 272
                               81.904 41.958 15.747 1.00 42.41
     ATOM
                               80.652 41.551 13.915 1.00 39.79
             902 N THR 273
     ATOM
                                79.492 42.282 14.401 1.00 38.82
             903 CA THR 273
45
     ATOM
                                79.334 43.648 13.670 1.00 39.73
     ATOM
             904 CB THR 273
                                 79.288 43.439 12.254 1.00 39.36
             905 OG1 THR 273
     ATOM
                                 80.496 44.578 13.991 1.00 41.31
             906 CG2 THR 273
     ATOM
                               78.203 41.485 14.211 1.00 38.36
             907 C THR 273
     ATOM
                               78.151 40.546 13.408 1.00 33.79
             908 O THR 273
50
     ATOM
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	ATO) (000 N I THE 274	77.187 41.835 14.995 1.00 36.91
	ATOM	909 N LEU 274	75.869 41.212 14.912 1.00 34.49
	ATOM	910 CA LEU 274	75.342 40.822 16.297 1.00 30.37
	ATOM	911 CB LEU 274	
_	ATOM	912 CG LEU 274	
5	ATOM	913 CD1 LEU 274	
	ATOM	914 CD2 LEU 274	75.749 38.341 16.318 1.00 26.86
	ATOM	915 C LEU 274	74.956 42.289 14.352 1.00 35.35
	ATOM	916 O LEU 274	75.171 43.478 14.601 1.00 37.47
	ATOM	917 N THR 275	73.942 41.890 13.599 1.00 34.05
10	ATOM	918 CA THR 275	73.020 42.868 13.052 1.00 32.62
	ATOM	919 CB THR 275	72.824 42.674 11.542 1.00 35.14
	ATOM	920 OG1 THR 275	74.108 42.590 10.909 1.00 39.50
	ATOM	921 CG2 THR 275	72.064 43.851 10.952 1.00 30.94
	ATOM	922 C THR 275	71.699 42.746 13.793 1.00 30.92
15	ATOM	923 O THR 275	71.100 41.670 13.845 1.00 36.53
	ATOM	924 N LEU 276	71.291 43.835 14.434 1.00 28.10
	ATOM	925 CA LEU 276	70.051 43.868 15.192 1.00 27.78
	ATOM	926 CB LEU 276	70.205 44.780 16.420 1.00 22.51
	ATOM	927 CG LEU 276	71.383 44.532 17.373 1.00 25.89
20	ATOM	928 CD1 LEU 276	71.225 45.408 18.608 1.00 20.70
	ATOM	929 CD2 LEU 276	71.456 43.069 17.782 1.00 20.79
	ATOM	930 C LEU 276	68.930 44.376 14.296 1.00 27.27
	ATOM	931 O LEU 276	69.068 45.430 13.672 1.00 29.06
	ATOM	932 N SER 277	67.854 43.598 14.187 1.00 25.97
25	ATOM	933 CA SER 277	66.697 43.957 13.366 1.00 28.63
	ATOM	934 CB SER 277	65.990 45.177 13.967 1.00 27.78
	ATOM	935 OG SER 277	65.561 44.905 15.290 1.00 22.65
	ATOM	936 C SER 277	67.067 44.209 11.897 1.00 30.31
	ATOM	937 O SER 277	66.374 44.939 11.181 1.00 28.52
30	ATOM	938 N GLY 278	68.168 43.597 11.465 1.00 31.24
20	ATOM	939 CA GLY 278	68.638 43.754 10.101 1.00 39.59
	ATOM	940 C GLY 278	68.999 45.178 9.706 1.00 44.55
	ATOM	941 O GLY 278	69.104 45.479 8.517 1.00 46.66
	ATOM	942 N GLU 279	69.234 46.046 10.686 1.00 43.47
35	ATOM	943 CA GLU 279	69.566 47.435 10.387 1.00 43.87
23	ATOM	944 CB GLU 279	68.314 48.312 10.515 1.00 44.28
	ATOM	945 CG GLU 279	67.703 48.322 11.908 1.00 52.30
	ATOM	946 CD GLU 279	66.440 49.159 12.001 1.00 60.23
	ATOM	947 OE1 GLU 279	66.398 50.074 12.853 1.00 63.06
40	ATOM	948 OE2 GLU 279	65.485 48.894 11.238 1.00 65.67
40	ATOM	949 C GLU 279	70.700 48.038 11.216 1.00 42.40
	ATOM	950 O GLU 279	71.330 49.001 10.787 1.00 43.89
	ATOM	951 N MET 280	70.977 47.472 12.388 1.00 40.86
	ATOM	951 N MET 280 952 CA MET 280	72.027 48.009 13.248 1.00 40.80
15	ATOM	952 CA MET 280 953 CB MET 280	71.435 48.415 14.603 1.00 29.25
45		953 CB MET 280 954 CG MET 280	72.384 49.193 15.506 1.00 27.23
	ATOM		71.830 49.235 17.232 1.00 34.02
	ATOM		70.566 50.495 17.197 1.00 26.56
	ATOM		73.172 47.033 13.465 1.00 32.77
50	ATOM	957 C MET 280	
50	ATOM	958 O MET 280	72.983 45.971 14.058 1.00 34.61

	ATOM	959 N ALA 281	74.351 47.375 12.959 1.00 31.87
	ATOM	960 CA ALA 281	75.523 46.526 13.147 1.00 34.71
	ATOM	961 CB ALA 281	76.519 46.727 12.023 1.00 34.42
	ATOM	962 C ALA 281	76.125 46.950 14.482 1.00 36.76
5	ATOM	963 O ALA 281	76.416 48.129 14.693 1.00 34.59
,	ATOM	964 N VAL 282	76.275 45.993 15.390 1.00 37.16
	ATOM	965 CA VAL 282	76.798 46.263 16.721 1.00 37.83
	ATOM	966 CB VAL 282	75.692 46.023 17.780 1.00 37.58
	ATOM	967 CG1 VAL 282	76.219 46.271 19.175 1.00 48.99
10		967 CG1 VAL 282 968 CG2 VAL 282	74.514 46.939 17.514 1.00 43.59
10	ATOM	968 CG2 VAL 282 969 C VAL 282	78.017 45.400 17.046 1.00 39.04
	ATOM		78.081 44.230 16.660 1.00 39.16
	ATOM		78.989 45.993 17.735 1.00 38.75
	ATOM	971 N LYS 283	80.205 45.287 18.136 1.00 42.18
	ATOM	972 CA LYS 283	81.428 46.208 18.045 1.00 47.46
15	ATOM	973 CB LYS 283	81.803 46.617 16.632 1.00 51.71
	ATOM	974 CG LYS 283	83.092 47.416 16.618 1.00 59.26
	ATOM	975 CD LYS 283	
	ATOM	976 CE LYS 283	83.481 47.813 15.202 1.00 62.52 82.492 48.742 14.588 1.00 66.27
20	ATOM	977 NZ LYS 283	80.075 44.746 19.559 1.00 38.78
20	ATOM	978 C LYS 283	79.283 45.257 20.356 1.00 40.63
	ATOM	979 O LYS 283	80.900 43.753 19.881 1.00 36.01
	ATOM	980 N ARG 284 981 CA ARG 284	80.908 43.104 21.189 1.00 38.62
	ATOM		82.150 42.224 21.327 1.00 38.83
25	ATOM	982 CB ARG 284	82.130 42.224 21.327 1.00 38.83 82.220 41.091 20.333 1.00 41.87
25	ATOM	983 CG ARG 284	83.521 40.335 20.451 1.00 39.60
	ATOM	984 CD ARG 284	83.506 39.120 19.644 1.00 45.18
	ATOM	985 NE ARG 284	83.259 37.905 20.128 1.00 44.79
	ATOM	986 CZ ARG 284 987 NH1 ARG 284	83.239 37.903 20.128 1.00 44.79
20	ATOM		83,271 36.852 19.319 1.00 42.27
30	ATOM	988 NH2 ARG 284	80.829 44.051 22.385 1.00 41.18
	ATOM	989 C ARG 284	79.995 43.867 23.274 1.00 44.38
	ATOM	990 O ARG 284	81.703 45.052 22.416 1.00 38.71
	ATOM	991 N GLU 285	81.724 46.002 23.525 1.00 37.18
2.5	ATOM	992 CA GLU 285	82.950 46.906 23.422 1.00 36.65
35	ATOM	993 CB GLU 285 994 C GLU 285	82.930 46.906 23.422 1.00 30.03
	ATOM		79.921 47.074 24.704 1.00 33.00
	ATOM	995 O GLU 285	79.921 47.074 24.704 1.00 33.00 79.920 47.245 22.463 1.00 32.01
	ATOM	996 N GLN 286	78.714 48.061 22.425 1.00 32.31
40	ATOM	997 CA GLN 286	
40	ATOM	998 CB GLN 286	78.440 48.525 20.997 1.00 38.24 79.565 49.352 20.392 1.00 42.42
	ATOM	999 CG GLN 286	79.277 49.761 18.964 1.00 44.79
	ATOM	1000 CD GLN 286	79.103 48.910 18.089 1.00 42.21
	ATOM	1001 OE1 GLN 286	
	ATOM	1002 NE2 GLN 286	
45	ATOM	1003 C GLN 286	77.484 47.355 23.002 1.00 33.08
	ATOM	1004 O GLN 286	76.770 47.929 23.827 1.00 30.95
	ATOM	1005 N LEU 287	77.245 46.114 22.579 1.00 31.49
	ATOM	1006 CA LEU 287	76.095 45.350 23.068 1.00 31.01
	ATOM	1007 CB LEU 287	75.892 44.073 22.242 1.00 24.63
50	ATOM	1008 CG LEU 287	74.498 43.780 21.661 1.00 27.34

	ATOM	1009 CD1 LEU 287	74.382 42.282 21.359 1.00 20.50
	ATOM	1010 CD2 LEU 287	73.393 44.205 22.616 1.00 14.41
	ATOM	1011 C LEU 287	76.298 44.986 24.538 1.00 32.80
	ATOM	1012 O LEU 287	75.351 45.014 25.334 1.00 32.10
5	ATOM	1013 N LYS 288	77.536 44.641 24.885 1.00 32.54
	ATOM	1014 CA LYS 288	77.897 44.280 26.251 1.00 30.70
	ATOM	1015 CB LYS 288	79.376 43.893 26.315 1.00 31.24
	ATOM	1016 CG LYS 288	79.834 43.382 27.662 1.00 34.69
	ATOM	1017 CD LYS 288	81.227 42.784 27.574 1.00 37.69
10	ATOM	1018 CE LYS 288	81.638 42.177 28.904 1.00 42.86
	ATOM	1019 NZ LYS 288	82.883 41.369 28.786 1.00 49.63
	ATOM	1020 C LYS 288	77.611 45.448 27.189 1.00 28.74
	ATOM	1021 O LYS 288	76.827 45.319 28.129 1.00 34.45
	ATOM	1022 N ASN 289	78.190 46.602 26.882 1.00 26.57
15	ATOM	1023 CA ASN 289	78.011 47.803 27.691 1.00 30.84
	ATOM	1024 CB ASN 289	79.012 48.879 27.274 1.00 26.04
	ATOM	1025 CG ASN 289	80.437 48.485 27.570 1.00 35.16
	ATOM	1026 OD1 ASN 289	80.700 47.718 28.499 1.00 42.54
	ATOM	1027 ND2 ASN 289	81.371 48.998 26.784 1.00 32.82
20	ATOM	1028 C ASN 289	76.602 48.371 27.620 1.00 35.05
	ATOM	1029 O ASN 289	76.154 49.039 28.550 1.00 36.94
	ATOM	1030 N GLY 290	75.909 48.113 26.515 1.00 32.43
	ATOM	1031 CA GLY 290	74.556 48.614 26.345 1.00 28.66
	ATOM	1032 C GLY 290	73.525 48.024 27.289 1.00 28.48
25	ATOM	1033 O GLY 290	72.377 48.467 27.308 1.00 28.17
	ATOM	1034 N GLY 291	73.908 47.002 28.047 1.00 28.66
	ATOM	1035 CA GLY 291	72.969 46.408 28.980 1.00 29.19
	ATOM	1036 C GLY 291	72.976 44.894 29.075 1.00 29.76
	ATOM	1037 O GLY 291	72.595 44.340 30.105 1.00 34.44
30	ATOM	1038 N LEU 292	73.399 44.213 28.017 1.00 29.69
	ATOM	1039 CA LEU 292	73.410 42.755 28.036 1.00 30.64
	ATOM	1040 CB LEU 292	73.421 42.194 26.611 1.00 27.07
	ATOM	1041 CG LEU 292	72.113 42.348 25.833 1.00 23.27
	ATOM	1042 CD1 LEU 292	72.202 41.580 24.532 1.00 22.24
35	ATOM	1043 CD2 LEU 292	70.950 41.827 26.661 1.00 23.80
	ATOM	1044 C LEU 292	74.530 42.125 28.861 1.00 29.22
	ATOM	1045 O LEU 292	74.365 41.033 29.404 1.00 31.02
	ATOM	1046 N GLY 293	75.671 42.800 28.945 1.00 30.26
	ATOM	1047 CA GLY 293	76.788 42.259 29.700 1.00 28.37
40	ATOM	1048 C GLY 293	77.307 40.995 29.040 1.00 29.85
	ATOM	1049 O GLY 293	77.460 40.951 27.820 1.00 32.37
	ATOM	1050 N VAL 294	77.537 39.953 29.832 1.00 30.08
	ATOM	1051 CA VAL 294	78.041 38.687 29.308 1.00 31.62
	ATOM	1052 CB VAL 294	78.466 37.716 30.442 1.00 29.11
45	ATOM	1053 CG1 VAL 294	79.649 38.292 31.191 1.00 31.37
	ATOM	1054 CG2 VAL 294	77.304 37.443 31.396 1.00 26.69
	ATOM	1055 C VAL 294	77.079 37.978 28.351 1.00 32.81
	ATOM	1056 O VAL 294	77.496 37.095 27.591 1.00 33.00
	ATOM	1057 N VAL 295	75.801 38.356 28.380 1.00 30.45
50	ATOM	1058 CA VAL 295	74.814 37.752 27.487 1.00 28.02

	ATOM	1059 CB VAL 295	73.378 38.232 27.793 1.00 29.96
	ATOM	1060 CG1 VAL 295	72.380 37.575 26.838 1.00 22.55
	ATOM	1061 CG2 VAL 295	73.016 37.903 29.232 1.00 20.10
	ATOM	1062 C VAL 295	75.203 38.115 26.057 1.00 29.90
5	ATOM	1063 O VAL 295	75.047 37.312 25.140 1.00 34.47
•	ATOM	1064 N SER 296	75.762 39.309 25.886 1.00 29.11
	ATOM	1065 CA SER 296	76.215 39.771 24.581 1.00 30.96
	ATOM	1066 CB SER 296	76.785 41.184 24.702 1.00 27.26
	ATOM	1067 OG SER 296	77.300 41.648 23.469 1.00 22.93
10	ATOM	1068 C SER 296	77.294 38.811 24.080 1.00 36.41
	ATOM	1069 O SER 296	77.238 38.341 22.939 1.00 38.84
	ATOM	1070 N ASP 297	78.254 38.501 24.954 1.00 35.29
	ATOM	1071 CA ASP 297	79.346 37.585 24.629 1.00 32.14
	ATOM	1072 CB ASP 297	80.245 37.356 25.851 1.00 36.57
15	ATOM	1073 CG ASP 297	80.958 38.616 26.307 1.00 41.75
	ATOM	1074 OD1 ASP 297	81.492 39.352 25.447 1.00 45.45
	ATOM	1075 OD2 ASP 297	80.999 38.861 27.532 1.00 45.15
	ATOM	1076 C ASP 297	78.768 36.249 24.191 1.00 29.61
	ATOM	1077 O ASP 297	79.242 35.644 23.231 1.00 32.90
20	ATOM	1078 N ALA 298	77.738 35.804 24.903 1.00 27.85
	ATOM	1079 CA ALA 298	77.071 34.544 24.608 1.00 27.89
	ATOM	1080 CB ALA 298	75.998 34.258 25.657 1.00 21.67
	ATOM	1081 C ALA 298	76.462 34.539 23.202 1.00 28.26
	ATOM	1082 O ALA 298	76.648 33.579 22.446 1.00 30.19
25	ATOM	1083 N ILE 299	75.744 35.606 22.853 1.00 25.20
	ATOM	1084 CA ILE 299	75.119 35.708 21.537 1.00 23.46
	ATOM	1085 CB ILE 299	74.200 36.944 21.427 1.00 21.63
	ATOM	1086 CG2 ILE 299	73.491 36.946 20.078 1.00 22.20
20	ATOM	1087 CG1 ILE 299	73.145 36.914 22.536 1.00 19.79 72.245 38.139 22.578 1.00 18.33
30	ATOM	1088 CD1 ILE 299	72.245 38.139 22.378 1.00 18.33 76.181 35.752 20.444 1.00 26.28
	ATOM	1089 C ILE 299 1090 O ILE 299	76.043 35.095 19.414 1.00 31.72
	ATOM		77.247 36.512 20.675 1.00 29.35
	ATOM ATOM	1091 N PHE 300 1092 CA PHE 300	78.338 36.613 19.709 1.00 29.01
35	ATOM	1092 CA PHE 300 1093 CB PHE 300	79,386 37.622 20.182 1.00 29.53
33	ATOM	1093 CB PHE 300	79.239 38.978 19.562 1.00 27.60
	ATOM	1094 CG PHE 300	78.481 39.964 20.179 1.00 24.86
	ATOM	1095 CD111E 300	79.853 39.266 18.350 1.00 27.39
	ATOM	1090 CB211E 300	78.337 41.218 19.597 1.00 25.66
40	ATOM	1097 CE1111E 300	79.715 40.518 17.761 1.00 25.97
40	ATOM	1090 CZ PHE 300	78.956 41.495 18.384 1.00 21.03
	ATOM	1100 C PHE 300	78.988 35.248 19.496 1.00 30.34
	ATOM	1101 O PHE 300	79.309 34.873 18.367 1.00 29.35
	ATOM	1102 N GLU 301	79.181 34.507 20.582 1.00 31.04
45	ATOM	1103 CA GLU 301	79.775 33.178 20.499 1.00 33.60
	ATOM	1104 CB GLU 301	80.012 32.607 21.898 1.00 31.64
	ATOM	1105 C GLU 301	78.851 32.265 19.696 1.00 33.90
	ATOM	1106 O GLU 301	79.315 31.473 18.872 1.00 33.33
	ATOM	1107 N LEU 302	77.546 32.386 19.935 1.00 31.13
50	ATOM	1108 CA LEU 302	76.556 31.581 19.227 1.00 27.57

	ATOM	1109 CB LEU 302	75.150 31.842 19.776 1.00 25.24
	ATOM	1110 CG LEU 302	73.994 31.131 19.059 1.00 28.59
	ATOM	1111 CD1 LEU 302	74.066 29.634 19.299 1.00 25.52
	ATOM	1112 CD2 LEU 302	72.660 31.682 19.532 1.00 19.30
5	ATOM	1113 C LEU 302	76.601 31.904 17.739 1.00 26.80
•	ATOM	1114 O LEU 302	76.682 31.003 16.904 1.00 27.81
	ATOM	1115 N GLY 303	76.576 33.195 17.416 1.00 26.47
	ATOM	1116 CA GLY 303	76.611 33.624 16.030 1.00 26.99
	ATOM	1117 C GLY 303	77.845 33.133 15.295 1.00 33.46
10	ATOM	1118 O GLY 303	77.757 32.646 14.164 1.00 32.33
10	ATOM	1119 N LYS 304	78.994 33.232 15.956 1.00 34.63
	ATOM	1120 CA LYS 304	80.269 32.813 15.383 1.00 36.20
	ATOM	1121 CB LYS 304	81.399 33.115 16.372 1.00 41.96
	ATOM	1122 CG LYS 304	82.779 33.179 15.757 1.00 47.05
15	ATOM	1122 CO LYS 304	83.800 33.610 16.796 1.00 59.47
15	ATOM	1124 CE LYS 304	85.179 33.791 16.181 1.00 65.89
	ATOM	1124 CE LTS 304 1125 NZ LYS 304	85.182 34.863 15.144 1.00 71.01
	ATOM	1126 C LYS 304	80.276 31.332 14.992 1.00 33.17
		1127 O LYS 304	80.752 30.974 13.913 1.00 34.44
20	ATOM	1128 N SER 305	79.739 30.482 15.861 1.00 31.40
20	ATOM ATOM	1129 CA SER 305	79.687 29.048 15.594 1.00 33.10
	ATOM	1130 CB SER 305	79.513 28.266 16.900 1.00 34.10
	ATOM	1131 OG SER 305	78.391 28.727 17.633 1.00 40.61
		1131 OG SER 303 1132 C SER 305	78.597 28.664 14.589 1.00 33.02
25	ATOM	1132 C SER 305	78.771 27.718 13.816 1.00 35.32
25	ATOM ATOM	1134 N LEU 306	77.488 29.404 14.580 1.00 32.14
	ATOM	1134 N LEU 300 1135 CA LEU 306	76.391 29.121 13.653 1.00 31.02
		1136 CB LEU 306	75.138 29.936 13.996 1.00 22.76
	ATOM	1137 CG LEU 306	74.361 29.487 15.235 1.00 24.42
20	ATOM ATOM	1137 CG LEU 306	73.094 30.311 15.380 1.00 23.13
30	ATOM	1138 CD1 LEU 300	74.016 28.009 15.126 1.00 25.53
	ATOM	1140 C LEU 306	76.780 29.354 12.198 1.00 33.11
		1140 C LEU 300 1141 O LEU 306	76.161 28.796 11.293 1.00 32.60
	ATOM ATOM	1141 O LEO 300 1142 N SER 307	77.821 30.153 11.975 1.00 36.12
25	ATOM	1142 N SER 307 1143 CA SER 307	78.296 30.448 10.624 1.00 38.80
35		1144 CB SER 307	79.514 31.373 10.677 1.00 41.64
	ATOM	1144 CB SER 307	79.224 32.556 11.401 1.00 54.66
	ATOM		78.650 29.182 9.845 1.00 36.98
	ATOM		78.302 29.055 8.669 1.00 42.87
40	ATOM		79.315 28.239 10.509 1.00 35.72
40	ATOM	1148 N ALA 308	79.719 26.983 9.879 1.00 32.70
	ATOM		80.683 26.227 10.782 1.00 33.88
	ATOM		78.531 26.093 9.521 1.00 34.83
	ATOM	1151 C ALA 308	78.620 25.278 8.600 1.00 39.61
4 ~	ATOM	1152 O ALA 308	77.424 26.250 10.244 1.00 31.54
45	ATOM		76.226 25.453 9.999 1.00 32.43
	ATOM		75.259 25.558 11.182 1.00 32.43
	ATOM		75.718 24.826 12.415 1.00 33.73
	ATOM	•	75.718 24.826 12.413 1.00 33.73 76.769 25.314 13.183 1.00 40.48
5 ^	ATOM		75.091 23.654 12.816 1.00 35.96
50	ATOM	1158 CD2 PHE 309	/3.091 23.034 12.810 1.00 33.90

	ATOM	1159 CE1 PHE 309	77.189 24.643 14.334 1.00 37.87
	ATOM	1160 CE2 PHE 309	75.502 22.975 13.962 1.00 38.44
	ATOM	1161 CZ PHE 309	76.553 23.471 14.722 1.00 37.34
	ATOM	1162 C PHE 309	75.507 25.809 8.693 1.00 34.76
5	ATOM	1163 O PHE 309	74.810 24.969 8.118 1.00 36.18
	ATOM	1164 N ASN 310	75.693 27.040 8.218 1.00 35.80
	ATOM	1165 CA ASN 310	75.060 27.506 6.980 1.00 41.00
	ATOM	1166 CB ASN 310	75.705 26.852 5.755 1.00 51.94
	ATOM	1167 CG ASN 310	77.053 27.452 5.419 1.00 67.92
10	ATOM	1168 OD1 ASN 310	77.139 28.439 4.687 1.00 77.32
	ATOM	1169 ND2 ASN 310	78.116 26.869 5.962 1.00 72.62
	ATOM	1170 C ASN 310	73.560 27.245 6.985 1.00 38.15
	ATOM	1171 O ASN 310	73.034 26.515 6.141 1.00 35.87
	ATOM	1172 N LEU 311	72.885 27.819 7.971 1.00 33.94
15	ATOM	1173 CA LEU 311	71.450 27.651 8.111 1.00 32.09
1.5	ATOM	1174 CB LEU 311	71.011 28.009 9.533 1.00 28.06
	ATOM	1175 CG LEU 311	71.656 27.301 10.724 1.00 26.38
	ATOM	1176 CD1 LEU 311	71.092 27.883 12.012 1.00 23.56
	ATOM	1177 CD2 LEU 311	71.409 25.801 10.651 1.00 21.24
20	ATOM	1178 C LEU 311	70.705 28.542 7.124 1.00 33.00
20	ATOM	1179 O LEU 311	71.173 29.630 6.782 1.00 35.47
	ATOM	1180 N ASP 312	69.569 28.057 6.638 1.00 27.78
	ATOM	1181 CA ASP 312	68.749 28.841 5.733 1.00 27.06
	ATOM	1182 CB ASP 312	68.385 28.049 4.456 1.00 25.84
25	ATOM	1183 CG ASP 312	67.580 26.778 4.724 1.00 25.67
	ATOM	1184 OD1 ASP 312	67.124 26.541 5.860 1.00 28.20
	ATOM	1185 OD2 ASP 312	67.387 26.008 3.762 1.00 27.62
	ATOM	1186 C ASP 312	67.517 29.314 6.514 1.00 28.51
	ATOM	1187 O ASP 312	67.371 28.990 7.703 1.00 25.35
30	ATOM	1188 N ASP 313	66.633 30.060 5.855 1.00 22.16
	ATOM	1189 CA ASP 313	65.430 30.589 6.494 1.00 21.37
	ATOM	1190 CB ASP 313	64.625 31.431 5.499 1.00 25.11
	ATOM	1191 CG ASP 313	65.380 32.666 5.025 1.00 31.54
	ATOM	1192 OD1 ASP 313	65.119 33.115 3.890 1.00 35.35
35	ATOM	1193 OD2 ASP 313	66.225 33.193 5.783 1.00 35.37
	ATOM	1194 C ASP 313	64.524 29.535 7.120 1.00 21.11
	ATOM	1195 O ASP 313	63.904 29.783 8.158 1.00 23.68
	ATOM	1196 N THR 314	64.440 28.367 6.489 1.00 22.88
	ATOM	1197 CA THR 314	63.591 27.281 6.981 1.00 22.81
40	ATOM	1198 CB THR 314	63.472 26.155 5.927 1.00 26.00
	ATOM	1199 OG1 THR 314	62.873 26.679 4.732 1.00 20.14
	ATOM	1200 CG2 THR 314	62.629 25.010 6.457 1.00 17.51
	ATOM	1201 C THR 314	64.086 26.706 8.310 1.00 19.46
	ATOM	1202 O THR 314	63.312 26.529 9.247 1.00 19.33
45	ATOM	1203 N GLU 315	65.381 26.431 8.392 1.00 17.49
	ATOM	1204 CA GLU 315	65.965 25.885 9.611 1.00 20.62
	ATOM	1205 CB GLU 315	67.426 25.514 9.358 1.00 14.39
	ATOM	1206 CG GLU 315	67.539 24.339 8.400 1.00 13.07
	ATOM	1207 CD GLU 315	68.923 24.125 7.835 1.00 14.98
50	ATOM	1208 OE1 GLU 315	69.634 25.116 7.552 1.00 17.71

	ATOM	1209 OE2 GLU 315	69.287 22.948 7.651 1.00 17.88
	ATOM	1210 C GLU 315	65.810 26.883 10.762 1.00 20.57
	ATOM	1211 O GLU 315	65.368 26.518 11.854 1.00 18.43
	ATOM	1212 N VAL 316	66.096 28.154 10.488 1.00 19.19
5	ATOM	1213 CA VAL 316	65.955 29.203 11.490 1.00 16.53
	ATOM	1214 CB VAL 316	66.418 30.567 10.933 1.00 17.42
	ATOM	1215 CG1 VAL 316	66.149 31.687 11.940 1.00 13.89
	ATOM	1216 CG2 VAL 316	67.900 30.506 10.594 1.00 14.31
	ATOM	1217 C VAL 316	64.488 29.291 11.927 1.00 19.53
10	ATOM	1217 C VAL 316	64.191 29.448 13.110 1.00 19.86
10	ATOM	1219 N ALA 317	63.575 29.159 10.970 1.00 19.02
	ATOM	1219 N ALA 317	62.145 29.215 11.254 1.00 16.95
	ATOM	1221 CB ALA 317	61.357 29.239 9.951 1.00 17.68
	ATOM	1221 CB ALA 317	61.674 28.047 12.126 1.00 14.13
15	ATOM	1223 O ALA 317	60.875 28.228 13.045 1.00 15.34
15	ATOM	1224 N LEU 318	62.154 26.847 11.819 1.00 17.41
	ATOM	1225 CA LEU 318	61.769 25.653 12.569 1.00 19.10
		1226 CB LEU 318	62.186 24.398 11.802 1.00 18.21
	ATOM		61.443 24.209 10.473 1.00 19.02
20	ATOM ATOM		62.105 23.128 9.646 1.00 16.10
20		1228 CD1 LEU 318 1229 CD2 LEU 318	59.987 23.875 10.735 1.00 11.32
	ATOM ATOM		62.399 25.685 13.954 1.00 22.38
	ATOM		61.782 25.278 14.945 1.00 21.64
		1231 O LEU 318 1232 N LEU 319	63.619 26.207 14.016 1.00 20.97
25	ATOM ATOM	1232 N LEU 319 1233 CA LEU 319	64.338 26.344 15.270 1.00 19.71
25	-	1234 CB LEU 319	65.715 26.951 15.005 1.00 20.56
	ATOM ATOM		66.722 27.036 16.152 1.00 32.05
		1235 CG LEU 319 1236 CD1 LEU 319	66.704 25.760 16.963 1.00 33.15
	ATOM ATOM		68.109 27.303 15.590 1.00 28.25
20			63.496 27.254 16.164 1.00 20.66
30	ATOM	1238 C LEU 319	63.215 26.920 17.313 1.00 24.47
	ATOM ATOM	1239 O LEU 319	63.026 28.365 15.604 1.00 19.25
		1240 N GLN 320 1241 CA GLN 320	62.191 29.307 16.346 1.00 19.02
	ATOM	1241 CA GLN 320 1242 CB GLN 320	61.842 30.526 15.488 1.00 19.11
25	ATOM		63.032 31.377 15.101 1.00 20.02
35	ATOM		62.665 32.562 14.224 1.00 23.65
	ATOM		62.663 32.362 14.224 1.00 23.03 63.487 33.445 13.997 1.00 22.68
	ATOM	1245 OE1 GLN 320	63.487 33.443 13.997 1.00 22.08 61.440 32.574 13.704 1.00 20.77
	ATOM	1246 NE2 GLN 320	60.905 28.635 16.811 1.00 20.52
40	ATOM	1247 C GLN 320	
40	ATOM	1248 O GLN 320	60.465 28.845 17.938 1.00 22.04
	ATOM	1249 N ALA 321	60.306 27.825 15.942 1.00 21.01
	ATOM	1250 CA ALA 321	59.069 27.128 16.280 1.00 16.83 58.556 26.358 15.079 1.00 16.58
	ATOM	1251 CB ALA 321	
4.5	ATOM	1252 C ALA 321	59.288 26.185 17.462 1.00 18.15
45	ATOM	1253 O ALA 321	58.427 26.069 18.344 1.00 13.03
	ATOM	1254 N VAL 322	60.442 25.523 17.481 1.00 14.89
	ATOM	1255 CA VAL 322	60.774 24.599 18.559 1.00 19.05
	ATOM	1256 CB VAL 322	62.051 23.779 18.233 1.00 21.50
.	ATOM	1257 CG1 VAL 322	62.510 22.990 19.457 1.00 21.49
50	ATOM	1258 CG2 VAL 322	61.773 22.819 17.073 1.00 15.42

ATOM 1260 O VAL 322 60.478 24.940 20.919 1.00 21.58 ATOM 1261 N LEU 323 61.591 26.537 19.788 1.00 20.25 ATOM 1262 CA LEU 323 61.804 27.387 20.959 1.00 19.3 ATOM 1263 CB LEU 323 62.683 28.586 20.597 1.00 12.9 ATOM 1264 CG LEU 323 64.129 28.273 20.217 1.00 20.7 ATOM 1265 CD1 LEU 323 64.805 29.503 19.641 1.00 13.2 ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.5 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08 ATOM 1270 CA LEU 324 58.248 28.753 20.944 1.00 21.2	5 2 5 0 23 91 5 4 5 7 33 9 90 5 5 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM 1262 CA LEU 323 61.804 27.387 20.959 1.00 19.3 5 ATOM 1263 CB LEU 323 62.683 28.586 20.597 1.00 12.9 ATOM 1264 CG LEU 323 64.129 28.273 20.217 1.00 20.7 ATOM 1265 CD1 LEU 323 64.805 29.503 19.641 1.00 13.2 ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.9 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	2 5 0 23 91 4 5 7 39
5 ATOM 1263 CB LEU 323 62.683 28.586 20.597 1.00 12.9 ATOM 1264 CG LEU 323 64.129 28.273 20.217 1.00 20.7 ATOM 1265 CD1 LEU 323 64.805 29.503 19.641 1.00 13.2 ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.5 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	5 0 223 991 8 8 4 5 7 7 39 90
ATOM 1264 CG LEU 323 64.129 28.273 20.217 1.00 20.7 ATOM 1265 CD1 LEU 323 64.805 29.503 19.641 1.00 13.2 ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.5 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	0 23 91 3 4 5 7 39 90
ATOM 1265 CD1 LEU 323 64.805 29.503 19.641 1.00 13.2 ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.5 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	23 91 3 4 5 7 39
ATOM 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.59 ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	91 3 4 5 7 39
ATOM 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	3 4 5 7 39
10 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	3 4 5 7 39
ATOM 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08	.4 5 7 39 90
ATOM 1270 CA LEU 324 58.248 28.753 20.944 1.00 21.2	5 7 39 90
	7 39 90
ATOM 1271 CB LEU 324 57.555 29.333 19.707 1.00 18.4	39 90
ATOM 1272 CG LEU 324 56.119 29.847 19.868 1.00 17.0	90
15 ATOM 1273 CD1 LEU 324 56.083 31.092 20.752 1.00 15.3	
ATOM 1274 CD2 LEU 324 55.545 30.162 18.498 1.00 17.9	
ATOM 1275 C LEU 324 57.342 27.706 21.598 1.00 21.54	
ATOM 1276 O LEU 324 56.742 27.967 22.642 1.00 23.41	
ATOM 1277 N MET 325 57.249 26.521 21.003 1.00 24.63	3
20 ATOM 1278 CA MET 325 56.380 25.476 21.545 1.00 25.3	
ATOM 1279 CB MET 325 55.901 24.536 20.430 1.00 25.5	
ATOM 1280 CG MET 325 55.235 25.220 19.232 1.00 21.8	
ATOM 1281 SD MET 325 53.871 26.337 19.649 1.00 25.5	-
ATOM 1282 CE MET 325 52.705 25.250 20.397 1.00 17.6	
25 ATOM 1283 C MET 325 57.031 24.676 22.675 1.00 27.58	
ATOM 1284 O MET 325 56.988 23.450 22.690 1.00 28.61	
ATOM 1285 N SER 326 57.613 25.376 23.638 1.00 27.98	
ATOM 1286 CA SER 326 58.265 24.718 24.757 1.00 31.60	
ATOM 1287 CB SER 326 59.527 25.493 25.155 1.00 35.80 30 ATOM 1288 OG SER 326 60.123 24.966 26.327 1.00 43.70	
30 ATOM 1288 OG SER 326 60.123 24.966 26.327 1.00 43.74 ATOM 1289 C SER 326 57.313 24.624 25.939 1.00 32.12	
ATOM 1289 C SER 326 57.313 24.024 23.939 1.00 32.12 ATOM 1290 O SER 326 56.590 25.574 26.240 1.00 30.91	
ATOM 1290 O SER 320 30.390 23.374 20.240 1.00 30.31 ATOM 1291 N THR 327 57.276 23.464 26.583 1.00 35.41	
ATOM 1292 CA THR 327 56.420 23.404 26.565 1.00 39.41	
35 ATOM 1293 CB THR 327 55.777 21.890 27.758 1.00 38.8	
ATOM 1294 OG1 THR 327 56.784 20.890 27.538 1.00 42.	
ATOM 1295 CG2 THR 327 54.716 21.802 26.679 1.00 40.	
ATOM 1296 C THR 327 57.232 23.471 29.022 1.00 43.86	
ATOM 1297 O THR 327 56.785 23.133 30.118 1.00 42.40	
40 ATOM 1298 N ASP 328 58.417 24.054 28.869 1.00 47.35	
ATOM 1299 CA ASP 328 59.309 24.308 29.987 1.00 49.4	
ATOM 1300 CB ASP 328 60.750 24.358 29.482 1.00 58.00	
ATOM 1301 CG ASP 328 61.718 23.687 30.425 1.00 72.10	6
ATOM 1302 OD1 ASP 328 61.816 24.117 31.595 1.00 82.3	
45 ATOM 1303 OD2 ASP 328 62.378 22.720 29.994 1.00 81.6	53
ATOM 1304 C ASP 328 58.951 25.625 30.676 1.00 47.99	
ATOM 1305 O ASP 328 59.830 26.373 31.093 1.00 53.33	
ATOM 1306 N ARG 329 57.657 25.910 30.780 1.00 48.33	
ATOM 1307 CA ARG 329 57.177 27.135 31.413 1.00 47.6	
50 ATOM 1308 CB ARG 329 56.562 28.091 30.379 1.00 47.6	هر

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ATOM 1309 CG ARG 329
                                57.550 28.802 29.450 1.00 47.87
                                57.893 27.968 28.226 1.00 44.00
     ATOM 1310 CD ARG 329
     ATOM 1311 NE ARG 329
                                58.759 28.682 27.288 1.00 41.17
                                60.087 28.605 27.283 1.00 48.58
     ATOM 1312 CZ ARG 329
     ATOM 1313 NH1 ARG 329
                                 60.719 27.848 28.172 1.00 52.94
                                 60.784 29.257 26.362 1.00 43.16
     ATOM 1314 NH2 ARG 329
                               56.126 26.778 32.457 1.00 48.01
     ATOM 1315 C ARG 329
                               55.573 25.677 32.437 1.00 50.22
     ATOM 1316 O ARG 329
     ATOM 1317 N SER 330
                               55.832 27.716 33.351 1.00 47.37
                                54.848 27.490 34.402 1.00 47.64
     ATOM 1318 CA SER 330
10
                               55.376 28.021 35.736 1.00 46.62
     ATOM 1319 CB SER 330
                               53.506 28.139 34.074 1.00 46.40
     ATOM 1320 C SER 330
                               53.460 29.252 33.548 1.00 48.49
     ATOM 1321 O SER 330
     ATOM 1322 N GLY 331
                               52.421 27.424 34.359 1.00 44.16
     ATOM 1323 CA GLY 331
                                51.090 27.956 34.123 1.00 41.44
15
     ATOM 1324 C GLY 331
ATOM 1325 O GLY 331
                               50.424 27.660 32.790 1.00 42.83
                               49.478 28.351 32.413 1.00 45.88
     ATOM 1326 N LEU 332
                               50.889 26.643 32.075 1.00 40.10
                                50.288 26.300 30.789 1.00 39.27
     ATOM 1327 CA LEU 332
                                51.301 25.596 29.885 1.00 37.42
20
     ATOM 1328 CB LEU 332
                                52.436 26.426 29.291 1.00 35.35
     ATOM 1329 CG LEU 332
     ATOM 1330 CD1 LEU 332
                                53.374 25.505 28.530 1.00 31.61
     ATOM 1331 CD2 LEU 332
                                51.875 27.511 28.376 1.00 31.82
     ATOM 1332 C LEU 332
                               49.058 25.415 30.951 1.00 39.32
25
     ATOM 1333 O LEU 332
                               49.060 24.467 31.738 1.00 42.74
                               48.009 25.730 30.202 1.00 37.62
     ATOM 1334 N LEU 333
     ATOM 1335 CA LEU 333
                                46.778 24.953 30.241 1.00 41.30
     ATOM 1336 CB LEU 333
                                45.586 25.835 29.852 1.00 43.52
     ATOM 1337 CG LEU 333
                                45.125 26.904 30.848 1.00 49.39
30
     ATOM 1338 CD1 LEU 333
                                44.296 27.970 30.142 1.00 46.19
     ATOM 1339 CD2 LEU 333
                                44.330 26.248 31.968 1.00 51.29
     ATOM 1340 C LEU 333
                               46.859 23.762 29.285 1.00 41.39
     ATOM 1341 O LEU 333
                               46.565 22.628 29.657 1.00 43.41
     ATOM 1342 N CYA 334
                                47.317 24.024 28.067 1.00 42.18
                                47.409 23.003 27.029 1.00 39.56
     ATOM 1343 CA CYA 334
35
     ATOM 1344 CB CYA 334
                                47.004 23.616 25.691 1.00 45.48
     ATOM 1345 SG CYA 334
                                45.517 24.616 25.785 1.00 51.57
                                44.187 22.808 25.555 1.00 90.90
     ATOM 1346 AS CYA 334
                                48.776 22.347 26.891 1.00 38.28
     ATOM 1347 C CYA 334
                                49.273 22.178 25.778 1.00 40.95
40
     ATOM 1348 O CYA 334
                               49.345 21.913 28.009 1.00 36.05
     ATOM 1349 N VAL 335
     ATOM 1350 CA VAL 335
                                50.661 21.278 28.006 1.00 35.78
     ATOM 1351 CB VAL 335
                                50.996 20.679 29.399 1.00 35.53
     ATOM 1352 CG1 VAL 335
                                 52.413 20.123 29.407 1.00 32.76
     ATOM 1353 CG2 VAL 335
                                 50.822 21.729 30.490 1.00 28.87
45
                               50.776 20.170 26.950 1.00 36.41
     ATOM 1354 C VAL 335
     ATOM 1355 O VAL 335
                               51.756 20.104 26.202 1.00 34.26
     ATOM 1356 N ASP 336
                               49.756 19.323 26.880 1.00 38.42
                               49.736 18.209 25.942 1.00 39.71
     ATOM 1357 CA ASP 336
                                48.485 17.359 26.179 1.00 51.53
50
     ATOM 1358 CB ASP 336
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	4 703 4	1250 GG ACD 226	48.534 16.028 25.452 1.00 65.98
	ATOM	1359 CG ASP 336	49.240 15.114 25.934 1.00 70.75
	ATOM	1360 OD1 ASP 336	47.858 15.891 24.406 1.00 72.15
	ATOM	1361 OD2 ASP 336	49.794 18.668 24.486 1.00 37.72
_	ATOM	1362 C ASP 336	
5	ATOM	1363 O ASP 336	50.686 18.259 23.733 1.00 32.08 48.858 19.532 24.100 1.00 33.78
	ATOM	1364 N LYS 337	48.797 20.040 22.731 1.00 28.00
	ATOM	1365 CA LYS 337	
	ATOM	1366 CB LYS 337	47.626 21.022 22.574 1.00 22.46
	ATOM	1367 C LYS 337	50.116 20.704 22.334 1.00 29.06 50.607 20.512 21.220 1.00 28.41
10	ATOM	1368 O LYS 337	
	ATOM	1369 N ILE 338	50.705 21.449 23.267 1.00 27.56 51.964 22.138 23.022 1.00 25.03
	ATOM	1370 CA ILE 338	
	ATOM	1371 CB ILE 338	52.274 23.149 24.144 1.00 19.49
	ATOM	1372 CG2 ILE 338	53.577 23.876 23.859 1.00 19.00
15	ATOM	1373 CG1 ILE 338	51.135 24.167 24.232 1.00 21.97
	ATOM	1374 CD1 ILE 338	51.277 25.175 25.348 1.00 26.67
	ATOM	1375 C ILE 338	53.119 21.153 22.826 1.00 29.97
	ATOM	1376 O ILE 338	53.935 21.328 21.914 1.00 31.00
	ATOM	1377 N GLU 339	53.165 20.100 23.642 1.00 33.52
20	ATOM	1378 CA GLU 339	54.213 19.080 23.516 1.00 35.34
	ATOM	1379 CB GLU 339	54.136 18.062 24.659 1.00 39.97
	ATOM	1380 CG GLU 339	54.653 18.585 25.986 1.00 53.23
	ATOM	1381 CD GLU 339	54.549 17.579 27.126 1.00 61.16
	ATOM	1382 OE1 GLU 339	53.602 16.759 27.131 1.00 64.30
25	ATOM	1383 OE2 GLU 339	55.412 17.622 28.031 1.00 57.76
	ATOM	1384 C GLU 339	54.091 18.353 22.178 1.00 31.63
	ATOM	1385 O GLU 339	55.086 18.123 21.491 1.00 28.96
	ATOM	1386 N LYS 340	52.861 18.006 21.810 1.00 30.95
••	ATOM	1387 CA LYS 340	52.602 17.313 20.554 1.00 31.58
30	ATOM	1388 CB LYS 340	51.121 16.966 20.438 1.00 31.83 53.057 18.159 19.358 1.00 29.84
	ATOM	1389 C LYS 340	
	ATOM	1390 O LYS 340	53.696 17.640 18.438 1.00 31.58 52.765 19.460 19.388 1.00 25.33
	ATOM	1391 N SER 341	52.765 19.460 19.388 1.00 25.33 53.165 20.351 18.297 1.00 23.92
26	ATOM	1392 CA SER 341	
35	ATOM	1393 CB SER 341	52.468 21.707 18.400 1.00 24.02 52.700 22.302 19.657 1.00 48.88
	ATOM	1394 OG SER 341	54.677 20.533 18.240 1.00 24.39
	ATOM	1395 C SER 341	55.254 20.593 17.150 1.00 24.71
	ATOM	1396 O SER 341	55.324 20.606 19.405 1.00 25.45
40	ATOM	1397 N GLN 342	
40	ATOM	1398 CA GLN 342	56.777 20.751 19.437 1.00 26.66
	ATOM	1399 CB GLN 342	57.311 20.975 20.853 1.00 22.77
	ATOM	1400 CG GLN 342	58.805 21.307 20.840 1.00 25.76
	ATOM	1401 CD GLN 342	59.427 21.371 22.214 1.00 28.46
	ATOM	1402 OE1 GLN 342	
45	ATOM	1403 NE2 GLN 342	
	ATOM	1404 C GLN 342	57.425 19.504 18.843 1.00 23.37
	ATOM	1405 O GLN 342	58.414 19.598 18.106 1.00 23.65
	ATOM	1406 N GLU 343	56.864 18.340 19.162 1.00 21.48
50	ATOM	1407 CA GLU 343	57.370 17.076 18.641 1.00 20.74 56.599 15.902 19.247 1.00 22.09
50	ATOM	1408 CB GLU 343	30.399 13.902 19.247 1.00 22.09

	ATOM	1409 C GLU 343	57.225 17.094 17.119 1.00 19.18
	ATOM	1410 O GLU 343	58.156 16.743 16.393 1.00 21.11
	ATOM	1411 N ALA 344	56.077 17.570 16.648 1.00 19.93
	ATOM	1412 CA ALA 344	55.803 17.662 15.217 1.00 20.20
5	ATOM	1413 CB ALA 344	54.411 18.216 14.989 1.00 16.46
_	ATOM	1414 C ALA 344	56.850 18.539 14.528 1.00 20.75
	ATOM	1415 O ALA 344	57.432 18.140 13.514 1.00 25.13
	ATOM	1416 N TYR 345	57.105 19.722 15.088 1.00 21.31
	ATOM	1417 CA TYR 345	58.107 20.631 14.531 1.00 15.93
10	ATOM	1418 CB TYR 345	58.127 21.969 15.282 1.00 17.29
	ATOM	1419 CG TYR 345	57.049 22.927 14.833 1.00 16.11
	ATOM	1420 CD1 TYR 345	56.017 23.296 15.689 1.00 9.93
	ATOM	1421 CE1 TYR 345	54.999 24.138 15.263 1.00 16.95
	ATOM	1422 CD2 TYR 345	57.041 23.431 13.531 1.00 19.84
15	ATOM	1423 CE2 TYR 345	56.026 24.276 13.094 1.00 17.13
	ATOM	1424 CZ TYR 345	55.005 24.622 13.963 1.00 18.12
	ATOM	1425 OH TYR 345	53.980 25.430 13.530 1.00 26.25
	ATOM	1426 C TYR 345	59.493 20.008 14.554 1.00 20.65
	ATOM	1427 O TYR 345	60.240 20.129 13.583 1.00 20.75
20	ATOM	1428 N LEU 346	59.832 19.337 15.655 1.00 22.14
	ATOM	1429 CA LEU 346	61.134 18.684 15.803 1.00 19.43
	ATOM	1430 CB LEU 346	61.267 18.041 17.186 1.00 19.92
	ATOM	1431 CG LEU 346	61.683 18.945 18.347 1.00 25.56
	ATOM	1432 CD1 LEU 346	61.440 18.244 19.677 1.00 22.06
25	ATOM	1433 CD2 LEU 346	63.147 19.332 18.197 1.00 17.62
	ATOM	1434 C LEU 346	61.359 17.635 14.723 1.00 19.30
	ATOM	1435 O LEU 346	62.441 17.560 14.142 1.00 22.84
	ATOM	1436 N LEU 347	60.337 16.826 14.456 1.00 25.17
	ATOM	1437 CA LEU 347	60.423 15.790 13.427 1.00 24.55
30	ATOM	1438 CB LEU 347	59.187 14.892 13.453 1.00 25.47
	ATOM	1439 CG LEU 347	59.256 13.654 14.345 1.00 30.65
	ATOM	1440 CD1 LEU 347	57.941 12.890 14.258 1.00 34.28
	ATOM	1441 CD2 LEU 347	60.416 12.765 13.908 1.00 28.26
	ATOM	1442 C LEU 347	60.584 16.400 12.042 1.00 24.00
35	ATOM	1443 O LEU 347	61.399 15.932 11.245 1.00 29.74 59.809 17.443 11.761 1.00 22.72
	ATOM	1444 N ALA 348	59.809 17.443 11.761 1.00 22.72
	ATOM	1445 CA ALA 348 1446 CB ALA 348	58.789 19.188 10.388 1.00 22.73
	ATOM		61,246 18.762 10.316 1.00 20.34
40	ATOM	1447 C ALA 348 1448 O ALA 348	61.881 18.633 9.274 1.00 23.94
40	ATOM ATOM	1448 O ALA 348 1449 N PHE 349	61.707 19.402 11.388 1.00 22.19
		1449 N PHE 349 1450 CA PHE 349	63.001 20.078 11.435 1.00 19.41
	ATOM	1450 CA PHE 349	63.185 20.701 12.832 1.00 17.45
	ATOM ATOM	1451 CB PHE 349	64.371 21.632 12.963 1.00 18.70
45	ATOM	1453 CD1 PHE 349	65.183 21.943 11.874 1.00 19.09
43	ATOM	1454 CD2 PHE 349	64.669 22.203 14.199 1.00 21.81
	ATOM	1455 CE1 PHE 349	66.270 22.811 12.012 1.00 21.49
	ATOM	1456 CE2 PHE 349	65.753 23.072 14.351 1.00 18.58
	ATOM	1457 CZ PHE 349	66.555 23.376 13.256 1.00 18.67
50	ATOM	1458 C PHE 349	64.110 19.071 11.136 1.00 20.96
20	ATOM	1450 C THE 547	5 IV 17.071 11.150 1.00 20.70

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	ATOM	1459 O PHE 349	64.967 19.311 10.283 1.00 25.19
	ATOM	1460 N GLU 350	64.076 17.935 11.824 1.00 23.96
	ATOM	1461 CA GLU 350	65.077 16.888 11.642 1.00 27.98
	ATOM	1462 CB GLU 350	64.794 15.721 12.591 1.00 28.90
5	ATOM	1463 CG GLU 350	65.738 14.542 12.413 1.00 39.36
	ATOM	1464 CD GLU 350	65.603 13.497 13.505 1.00 41.62
	ATOM	1465 OE1 GLU 350	64.475 13.260 13.988 1.00 43.67
	ATOM	1466 OE2 GLU 350	66.636 12.908 13.876 1.00 49.64
	ATOM	1467 C GLU 350	65.100 16.385 10.203 1.00 27.12
10	ATOM	1468 O GLU 350	66.158 16.288 9.577 1.00 27.44
	ATOM	1469 N HIS 351	63.918 16.088 9.678 1.00 27.36
	ATOM	1470 CA HIS 351	63.787 15.591 8.318 1.00 23.97
	ATOM	1471 CB HIS 351	62.366 15.087 8.090 1.00 22.89
	ATOM	1472 CG HIS 351	61.991 13.945 8.986 1.00 24.58
15	ATOM	1473 CD2 HIS 351	62.736 13.209 9.846 1.00 25.83
13	ATOM	1474 ND1 HIS 351	60,709 13,448 9.073 1.00 26.50
	ATOM	1474 ND1 HIS 351	60.677 12.460 9.948 1.00 24.81
	ATOM	1476 NE2 HIS 351	61.896 12.295 10.431 1.00 28.42
	ATOM	1477 C HIS 351	64.200 16.635 7.278 1.00 24.22
20	ATOM	1477 C HIS 351	64.757 16.287 6.236 1.00 25.79
20		1478 O HIS 331 1479 N TYR 352	63.969 17.912 7.572 1.00 21.04
	ATOM		64.363 18.974 6.654 1.00 18.98
	ATOM		63.770 20.321 7.067 1.00 17.08
	ATOM		64.127 21.413 6.090 1.00 21.83
25	ATOM	1482 CG TYR 352	
25	ATOM	1483 CD1 TYR 352	
	ATOM	1484 CE1 TYR 352	
	ATOM	1485 CD2 TYR 352	
	ATOM	1486 CE2 TYR 352	
	ATOM	1487 CZ TYR 352	64.942 23.313 4.203 1.00 24.80
30	ATOM	1488 OH TYR 352	65.380 24.221 3.269 1.00 26.74
	ATOM	1489 C TYR 352	65.889 19.055 6.624 1.00 20.58
	ATOM	1490 O TYR 352	66.492 19.276 5.570 1.00 22.72
	ATOM	1491 N VAL 353	66.508 18.877 7.789 1.00 28.34
	ATOM	1492 CA VAL 353	67.967 18.892 7.904 1.00 22.38
35	ATOM	1493 CB VAL 353	68.419 18.755 9.389 1.00 26.46
	ATOM	1494 CG1 VAL 353	69.915 18.527 9.478 1.00 20.92
	ATOM	1495 CG2 VAL 353	68.053 20.009 10.165 1.00 22.46
	ATOM	1496 C VAL 353	68.518 17.725 7.078 1.00 23.51
	ATOM	1497 O VAL 353	69.535 17.865 6.391 1.00 24.73
40	ATOM	1498 N ASN 354	67.850 16.575 7.158 1.00 20.93
	ATOM	1499 CA ASN 354	68.252 15.392 6.397 1.00 27.25
	ATOM	1500 CB ASN 354	67.320 14.210 6.680 1.00 28.43
	ATOM	1501 CG ASN 354	67.521 13.607 8.058 1.00 31.50
	ATOM	1502 OD1 ASN 354	68.565 13.787 8.692 1.00 37.79
45	ATOM	1503 ND2 ASN 354	66.521 12.867 8.524 1.00 26.44
	ATOM	1504 C ASN 354	68.182 15.721 4.908 1.00 31.27
	ATOM	1505 O ASN 354	69.066 15.347 4.134 1.00 34.22
	ATOM	1506 N HIS 355	67.124 16.429 4.520 1.00 30.49
	ATOM	1507 CA HIS 355	66.917 16.826 3.132 1.00 26.88
50	ATOM		65.548 17.494 2.975 1.00 27.27

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65.319 18.103 1.625 1.00 37.76
    ATOM 1509 CG HIS 355
    ATOM 1510 CD2 HIS 355
                               65.439 19.382 1.196 1.00 35.28
                               64.913 17.369 0.532 1.00 34.93
    ATOM 1511 ND1 HIS 355
                               64.789 18.169 -0.513 1.00 34.84
    ATOM 1512 CE1 HIS 355
                               65.104 19.394 -0.135 1.00 33.13
    ATOM 1513 NE2 HIS 355
                              68.016 17.748 2.610 1.00 24.66
    ATOM 1514 C HIS 355
                              68.420 17.630 1.456 1.00 26.62
    ATOM 1515 O HIS 355
                               68.487 18.670 3.448 1.00 25.86
    ATOM 1516 N ARG 356
                                69.536 19.608 3.040 1.00 26.94
    ATOM 1517 CA ARG 356
                                69.620 20.791 3.996 1.00 20.57
10
    ATOM 1518 CB ARG 356
                                68.453 21.727 3.899 1.00 19.69
    ATOM 1519 CG ARG 356
                                68.866 23.110 4.340 1.00 23.81
    ATOM 1520 CD ARG 356
                                69.768 23.746 3.388 1.00 23.14
    ATOM 1521 NE ARG 356
    ATOM 1522 CZ ARG 356
                                70.641 24.697 3.702 1.00 24.11
    ATOM 1523 NH1 ARG 356
                                70.755 25.129 4.949 1.00 26.29
15
                                 71.384 25.242 2.754 1.00 32.79
    ATOM 1524 NH2 ARG 356
                               70.921 19.002 2.875 1.00 29.38
    ATOM 1525 C ARG 356
                               71.795 19.607 2.257 1.00 32.91
    ATOM 1526 O ARG 356
                               71.133 17.848 3.498 1.00 33.39
    ATOM 1527 N LYS 357
                               72.401 17.128 3.417 1.00 35.97
    ATOM 1528 CA LYS 357
20
                               72.479 16.363 2.089 1.00 40.55
    ATOM 1529 CB LYS 357
                                71.327 15.381 1.891 1.00 44.03
    ATOM 1530 CG LYS 357
                                71.360 14.722 0.523 1.00 52.31
    ATOM 1531 CD LYS 357
                               70.171 13.787 0.343 1.00 56.99
     ATOM 1532 CE LYS 357
                               70.208 13.085 -0.970 1.00 64.78
     ATOM 1533 NZ LYS 357
25
                               73.657 17.981 3.629 1.00 38.55
     ATOM 1534 C LYS 357
                               74.518 18.079 2.748 1.00 42.50
     ATOM 1535 O LYS 357
                              73.751 18.601 4.802 1.00 35.00
     ATOM 1536 N HIS 358
     ATOM 1537 CA HIS 358
                               74.906 19.418 5.155 1.00 32.94
                               74.732 20.018 6.552 1.00 27.62
     ATOM 1538 CB HIS 358
30
     ATOM 1539 CG HIS 358
                               73.669 21.067 6.643 1.00 26.64
                                72.330 20.968 6.819 1.00 20.85
     ATOM 1540 CD2 HIS 358
                                73.950 22.416 6.587 1.00 24.71
     ATOM 1541 ND1 HIS 358
                               72.831 23.103 6.724 1.00 21.02
     ATOM 1542 CE1 HIS 358
                               71.834 22.248 6.865 1.00 21.42
     ATOM 1543 NE2 HIS 358
35
                              76.140 18.520 5.176 1.00 36.60
     ATOM 1544 C HIS 358
                               76.072 17.379 5.635 1.00 38.73
     ATOM 1545 O HIS 358
                               77.267 19.037 4.702 1.00 41.40
     ATOM 1546 N ASN 359
                                78.515 18.277 4.689 1.00 45.02
     ATOM 1547 CA ASN 359
                                79.441 18.799 3.587 1.00 42.57
     ATOM 1548 CB ASN 359
40
                               79.193 18.386 6.058 1.00 46.59
     ATOM 1549 C ASN 359
     ATOM 1550 O ASN 359
                               80.405 18.588 6.150 1.00 52.31
                               78.400 18.254 7.117 1.00 45.14
     ATOM 1551 N ILE 360
                               78.896 18.348 8.487 1.00 43.69
     ATOM 1552 CA ILE 360
                               78.330 19.597 9.207 1.00 40.08
     ATOM 1553 CB ILE 360
45
                                78.824 19.657 10.645 1.00 32.11
     ATOM 1554 CG2 ILE 360
                                78.733 20.864 8.452 1.00 41.47
     ATOM 1555 CG1 ILE 360
                                78.057 22.115 8.954 1.00 44.93
     ATOM 1556 CD1 ILE 360
                              78,452 17.101 9.242 1.00 43.63
     ATOM 1557 C ILE 360
                              77.257 16.797 9.313 1.00 45.20
     ATOM 1558 O ILE 360
50
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ATOM 1559 N PRO 361
                                79.413 16.337 9.780 1.00 43.91
     ATOM 1560 CD PRO 361
                                80.871 16.540 9.699 1.00 47.07
     ATOM 1561 CA PRO 361
                                79.087 15.118 10.526 1.00 41.66
                                80.462 14.495 10.782 1.00 43.73
     ATOM 1562 CB PRO 361
     ATOM 1563 CG PRO 361
                                81.383 15.679 10.830 1.00 45.45
     ATOM 1564 C PRO 361
                               78.332 15.403 11.832 1.00 36.42
     ATOM 1565 O PRO 361
                               78.679 16.325 12.572 1.00 35.74
     ATOM 1566 N HIS 362
                               77.291 14.610 12.088 1.00 33.14
     ATOM 1567 CA HIS 362
                               76,462 14,726 13,292 1,00 34,09
                                77.288 14.413 14.547 1.00 33.82
     ATOM 1568 CB HIS 362
10
                                78.132 13.181 14.424 1.00 36.04
     ATOM 1569 CG HIS 362
                                77.793 11.885 14.224 1.00 34.77
     ATOM 1570 CD2 HIS 362
     ATOM 1571 ND1 HIS 362
                                79.509 13.212 14.482 1.00 37.16
                                79.983 11.990 14.325 1.00 37.16
     ATOM 1572 CE1 HIS 362
                                78.962 11.165 14.167 1.00 40.13
15
     ATOM 1573 NE2 HIS 362
     ATOM 1574 C HIS 362
                               75.829 16.110 13.417 1.00 31.00
     ATOM 1575 O HIS 362
                               75.617 16.608 14.525 1.00 30.22
     ATOM 1576 N PHE 363
                               75.478 16.690 12.272 1.00 33.06
     ATOM 1577 CA PHE 363
                                74.878 18.021 12.200 1.00 28.08
                                74.503 18.355 10.747 1.00 25.26
20
     ATOM 1578 CB PHE 363
     ATOM 1579 CG PHE 363
                                73.923 19.733 10.567 1.00 24.91
                                74.750 20.817 10.320 1.00 27.60
     ATOM 1580 CD1 PHE 363
     ATOM 1581 CD2 PHE 363
                                72.552 19.948 10.664 1.00 25.52
                                74.221 22.100 10.175 1.00 29.70
     ATOM 1582 CE1 PHE 363
     ATOM 1583 CE2 PHE 363
                                72.014 21.227 10.522 1.00 25.88
25
     ATOM 1584 CZ PHE 363
                                72.850 22.304 10.278 1.00 21.49
                               73.659 18.201 13.099 1.00 23.79
     ATOM 1585 C PHE 363
     ATOM 1586 O PHE 363
                               73.587 19.164 13.863 1.00 24.48
     ATOM 1587 N TRP 364
                               72.707 17.277 13.012 1.00 23.13
     ATOM 1588 CA TRP 364
                                71.484 17.369 13.805 1.00 25.06
30
                                70.536 16.201 13.494 1.00 21.17
     ATOM 1589 CB TRP
                          364
     ATOM 1590 CG TRP 364
                                69.247 16.220 14.271 1.00 23.14
     ATOM 1591 CD2 TRP 364
                                68.261 17.266 14.296 1.00 27.68
     ATOM 1592 CE2 TRP 364
                                67.229 16.845 15.165 1.00 28.31
35
     ATOM 1593 CE3 TRP
                          364
                                68.149 18.517 13.671 1.00 26.46
     ATOM 1594 CD1 TRP 364
                                68.784 15.241 15.096 1.00 23.76
     ATOM 1595 NE1 TRP 364
                                67.576 15.607 15.637 1.00 32.12
     ATOM 1596 CZ2 TRP 364
                                66.100 17.628 15.427 1.00 25.63
     ATOM 1597 CZ3 TRP 364
                                67.028 19.294 13.931 1.00 25.55
40 ATOM 1598 CH2 TRP 364
                                66.017 18.845 14.803 1.00 29.79
     ATOM 1599 C TRP 364
                               71.715 17.531 15.312 1.00 27.80
     ATOM 1600 O TRP 364
                               71.212 18.486 15.904 1.00 26.96
     ATOM 1601 N PRO 365
                               72.458 16.605 15.955 1.00 30.69
     ATOM 1602 CD PRO 365
                                72.974 15.308 15.481 1.00 31.45
45
     ATOM 1603 CA PRO 365
                                72.687 16.757 17.397 1.00 27.97
     ATOM 1604 CB PRO 365
                                73.506 15.512 17.752 1.00 26.50
     ATOM 1605 CG PRO 365
                                73.057 14.509 16.757 1.00 33.47
     ATOM 1606 C PRO 365
                               73.457 18.043 17.709 1.00 27.10
     ATOM 1607 O PRO 365
                               73.154 18.736 18.681 1.00 26.88
     ATOM 1608 N LYS 366
50
                               74.440 18.365 16.873 1.00 26.99
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	ATOM	1609 CA LYS 366	75.230 19.577 17.061 1.00 30.69
	ATOM	1610 CB LYS 366	76.275 19.708 15.957 1.00 28.53
	ATOM	1611 CG LYS 366	77.481 18.804 16.106 1.00 28.89
	ATOM	1612 CD LYS 366	78.430 19.027 14.939 1.00 32.51
5	ATOM	1613 CE LYS 366	79.743 18.294 15.116 1.00 38.52
	ATOM	1614 NZ LYS 366	80.632 18.506 13.939 1.00 45.28
	ATOM	1615 C LYS 366	74.349 20.831 17.079 1.00 36.18
	ATOM	1616 O LYS 366	74.472 21.672 17.972 1.00 39.82
	ATOM	1617 N LEU 367	73.464 20.950 16.091 1.00 37.54
10	ATOM	1618 CA LEU 367	72.557 22.092 15.994 1.00 36.14
	ATOM	1619 CB LEU 367	71.803 22.070 14.659 1.00 32.20
	ATOM	1620 CG LEU 367	70.764 23.179 14.447 1.00 36.16
	ATOM	1621 CD1 LEU 367	71.402 24.567 14.618 1.00 20.60
	ATOM	1622 CD2 LEU 367	70.139 23.030 13.065 1.00 34.30
15	ATOM	1623 C LEU 367	71.561 22.060 17.143 1.00 36.84
13	ATOM	1624 O LEU 367	71.231 23.091 17.729 1.00 36.94
	ATOM	1625 N LEU 368	71.083 20.866 17.459 1.00 37.81
	ATOM	1626 CA LEU 368	70.130 20.683 18.536 1.00 34.83
	ATOM	1627 CB LEU 368	69.763 19.205 18.622 1.00 36.98
20	ATOM	1628 CG LEU 368	68.421 18.777 19.205 1.00 40.34
20	ATOM	1629 CD1 LEU 368	67.276 19.595 18.619 1.00 36.28
	ATOM	1630 CD2 LEU 368	68.241 17.299 18.908 1.00 39.39
	ATOM	1631 C LEU 368	70.755 21.182 19.843 1.00 38.32
	ATOM	1632 O LEU 368	70.059 21.711 20.707 1.00 41.87
25	ATOM	1633 N MET 369	72.075 21.057 19.962 1.00 39.46
23	ATOM	1634 CA MET 369	72.790 21.515 21.154 1.00 40.12
	ATOM	1635 CB MET 369	74.219 20.971 21.168 1.00 41.26
	ATOM	1636 CG MET 369	74.307 19.493 21.521 1.00 47.83
	ATOM	1637 SD MET 369	75.961 18.810 21.289 1.00 55.72
30	ATOM	1638 CE MET 369	76.809 19.474 22.727 1.00 54.37
50	ATOM	1639 C MET 369	72.805 23.039 21.251 1.00 42.81
	ATOM	1640 O MET 369	72.990 23.601 22.335 1.00 47.81
	ATOM	1641 N LYS 370	72.622 23.708 20.115 1.00 40.09
	ATOM	1642 CA LYS 370	72.588 25.165 20.080 1.00 33.65
35	ATOM	1643 CB LYS 370	72.751 25.677 18.650 1.00 30.83
55	ATOM	1644 CG LYS 370	74.138 25.435 18.078 1.00 30.98
	ATOM	1645 CD LYS 370	75.188 26.198 18.867 1.00 37.82
	ATOM	1646 CE LYS 370	76.591 25.938 18.351 1.00 36.05
	ATOM	1647 NZ LYS 370	77.034 24.562 18.667 1.00 48.68
40	ATOM	1648 C LYS 370	71.293 25.684 20.702 1.00 33.32
	ATOM	1649 O LYS 370	71.218 26.842 21.112 1.00 34.75
	ATOM	1650 N VAL 371	70.277 24.826 20.779 1.00 31.90
	ATOM	1651 CA VAL 371	69.006 25.197 21.395 1.00 31.77
	ATOM	1652 CB VAL 371	67.933 24.092 21.214 1.00 30.28
45	ATOM	1653 CG1 VAL 371	66.673 24.429 21.995 1.00 30.02
73	ATOM	1654 CG2 VAL 371	67.596 23.933 19.746 1.00 32.23
	ATOM	1655 C VAL 371	69.277 25.417 22.885 1.00 34.44
	ATOM	1656 O VAL 371	68.722 26.331 23.499 1.00 33.35
	ATOM	1657 N THR 372	70.161 24.590 23.443 1.00 33.15
50	ATOM	1658 CA THR 372	70.551 24.675 24.847 1.00 32.47
		5/2	

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71.541 23.556 25.207 1.00 32.11
    ATOM 1659 CB THR 372
                                70.955 22.288 24.891 1.00 35.33
    ATOM 1660 OG1 THR 372
    ATOM 1661 CG2 THR 372
                                 71.894 23.603 26.688 1.00 32.54
                               71.226 26.020 25.108 1.00 34.49
    ATOM 1662 C THR 372
    ATOM 1663 O THR 372
                               70.936 26.696 26.099 1.00 34.07
    ATOM 1664 N ASP 373
                               72.120 26.405 24.202 1.00 32.77
                               72.830 27.671 24.315 1.00 28.08
    ATOM 1665 CA ASP 373
                               73.803 27.841 23.147 1.00 31.59
    ATOM 1666 CB ASP 373
                                74.910 26.789 23.142 1.00 37.29
    ATOM 1667 CG ASP 373
                                75.170 26.169 24.196 1.00 40.82
    ATOM 1668 OD1 ASP 373
10
                                75.531 26.586 22.079 1.00 40.81
    ATOM 1669 OD2 ASP 373
                               71.830 28.821 24.353 1.00 29.21
    ATOM 1670 C ASP 373
    ATOM 1671 O ASP 373
                               71.931 29.709 25.200 1.00 31.85
                               70.843 28.775 23.463 1.00 24.71
    ATOM 1672 N LEU 374
                                69.813 29.802 23.403 1.00 25.25
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    ATOM 1673 CA LEU 374
                                68,906 29.587 22.188 1.00 25.61
    ATOM 1674 CB LEU 374
                                69.480 30.084 20.858 1.00 25.51
           1675 CG LEU 374
    ATOM
    ATOM 1676 CD1 LEU 374
                                68.741 29.469 19.677 1.00 23.53
    ATOM 1677 CD2 LEU 374
                                69.405 31.596 20.820 1.00 21.92
                               68.994 29.827 24.686 1.00 26.84
    ATOM 1678 C LEU 374
20
                               68.591 30.895 25.151 1.00 28.96
    ATOM 1679 O LEU 374
                               68.746 28.651 25.254 1.00 31.00
    ATOM 1680 N ARG 375
    ATOM 1681 CA ARG 375
                                67.996 28.554 26.502 1.00 32.86
                                67.831 27.090 26.924 1.00 36.80
    ATOM 1682 CB ARG 375
                                66.861 26.297 26.071 1.00 44.91
    ATOM 1683 CG ARG 375
25
                                65.433 26.731 26.338 1.00 58.99
    ATOM 1684 CD ARG 375
                                64,501 26,210 25,342 1.00 72,26
    ATOM 1685 NE ARG 375
                                63.909 25.020 25.404 1.00 77.46
    ATOM 1686 CZ ARG 375
                                 64.147 24.201 26.422 1.00 80.94
    ATOM 1687 NH1 ARG 375
    ATOM 1688 NH2 ARG 375
                                 63.062 24.657 24.447 1.00 75.58
30
                               68.771 29.317 27.570 1.00 32.27
     ATOM 1689 C ARG 375
                                68.199 30.125 28.304 1.00 33.75
    ATOM 1690 O ARG 375
                                70.084 29.098 27.602 1.00 32.65
     ATOM 1691 N MET 376
                                70.967 29.753 28.560 1.00 35.83
     ATOM 1692 CA MET 376
35
     ATOM 1693 CB MET 376
                                72.392 29.210 28.434 1.00 39.25
                                72.526 27.751 28.839 1.00 54.45
     ATOM 1694 CG MET 376
     ATOM 1695 SD MET 376
                                74.245 27.212 28.944 1.00 73.93
    ATOM 1696 CE MET 376
                                74.421 26.270 27.434 1.00 67.01
    ATOM 1697 C MET 376
                               70.960 31.267 28.378 1.00 35.38
     ATOM 1698 O MET 376
                               70.882 32.015 29.353 1.00 34.73
40
                               71.038 31.716 27.129 1.00 32.51
     ATOM 1699 N ILE 377
                               71.016 33.142 26.816 1.00 26.55
     ATOM 1700 CA ILE 377
     ATOM 1701 CB ILE 377
                               71.182 33.370 25.299 1.00 24.84
     ATOM 1702 CG2 ILE 377
                                70.817 34.797 24.923 1.00 26.63
                                72.616 33.038 24.890 1.00 20.66
45
     ATOM 1703 CG1 ILE 377
                                72.872 33.104 23.409 1.00 20.74
     ATOM 1704 CD1 ILE 377
                              69.706 33.755 27.313 1.00 25.47
     ATOM 1705 C ILE 377
     ATOM 1706 O ILE 377
                               69.696 34.848 27.881 1.00 29.99
                               68.608 33.033 27.127 1.00 25.11
     ATOM 1707 N GLY 378
     ATOM 1708 CA GLY 378
                                67.321 33.522 27.580 1.00 27.82
50
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	ATOM	1709 C GLY 378 67.279 33.613 29.095 1.00 30.90
	ATOM	1710 O GLY 378 66.749 34.579 29.651 1.00 31.19
	ATOM	1711 N ALA 379 67.851 32.611 29.761 1.00 31.62
	ATOM	1712 CA ALA 379 67.896 32.547 31.223 1.00 30.74
5	ATOM	1713 CB ALA 379 68.433 31.198 31.671 1.00 30.82
-	ATOM	1714 C ALA 379 68.756 33.668 31.801 1.00 30.07
	ATOM	1715 O ALA 379 68.327 34.384 32.708 1.00 31.05
	ATOM	1716 N CYA 380 69.966 33.817 31.273 1.00 29.72
	ATOM	1717 CA CYA 380 70.873 34.866 31.723 1.00 33.36
10	ATOM	1718 CB CYA 380 72.201 34.809 30.963 1.00 38.31
	ATOM	1719 SG CYA 380 73.249 33.407 31.386 1.00 50.99
	ATOM	1720 AS CYA 380 74.982 33.655 29.929 1.00 70.37
	ATOM	1721 C CYA 380 70.226 36.232 31.535 1.00 33.40
	ATOM	1722 O CYA 380 70.246 37.062 32.442 1.00 36.41
15	ATOM	1723 N HIS 381 69.615 36.456 30.374 1.00 32.55
	ATOM	1724 CA HIS 381 68.965 37.734 30.114 1.00 26.41
	ATOM	1725 CB HIS 381 68.434 37.811 28.681 1.00 20.89
	ATOM	1726 CG HIS 381 67.593 39.023 28.423 1.00 15.78
	ATOM	1727 CD2 HIS 381 67.928 40.277 28.041 1.00 12.67
20	ATOM	1728 ND1 HIS 381 66.226 39.031 28.605 1.00 17.88
	ATOM	1729 CE1 HIS 381 65.756 40.239 28.353 1.00 16.27
	ATOM	1730 NE2 HIS 381 66.768 41.013 28.008 1.00 17.18
	ATOM	1731 C HIS 381 67.839 38.023 31.102 1.00 26.73
	ATOM	1732 O HIS 381 67.621 39.176 31.464 1.00 30.46
25	ATOM	1733 N ALA 382 67.111 36.991 31.521 1.00 26.68
	ATOM	1734 CA ALA 382 66.010 37.176 32.464 1.00 27.90
	ATOM	1735 CB ALA 382 65.237 35.878 32.642 1.00 25.29
	ATOM	1736 C ALA 382 66.511 37.697 33.810 1.00 31.23
	ATOM	1737 O ALA 382 65.927 38.617 34.378 1.00 37.67
30	ATOM	1738 N SER 383 67.596 37.114 34.316 1.00 34.15
	ATOM	1739 CA SER 383 68.174 37.550 35.588 1.00 37.23
	ATOM	1740 CB SER 383 69.294 36.605 36.027 1.00 40.21
	ATOM	1741 OG SER 383 68.785 35.324 36.361 1.00 53.99
	ATOM	1742 C SER 383 68.727 38.958 35.417 1.00 33.67
35	ATOM	1743 O SER 383 68.532 39.827 36.268 1.00 40.73
	ATOM	1744 N ARG 384 69.411 39.171 34.298 1.00 29.95
	ATOM	1745 CA ARG 384 70.000 40.458 33.957 1.00 29.77
	ATOM	1746 CB ARG 384 70.684 40.350 32.594 1.00 30.79
	ATOM	1747 CG ARG 384 71.481 41.558 32.167 1.00 31.34
40	ATOM	1748 CD ARG 384 72.781 41.638 32.918 1.00 33.62
	ATOM	1749 NE ARG 384 73.657 42.660 32.358 1.00 41.68
	ATOM	1750 CZ ARG 384 74.584 43.310 33.052 1.00 41.20
	ATOM	1751 NH1 ARG 384 74.756 43.047 34.339 1.00 42.11
	ATOM	1752 NH2 ARG 384 75.349 44.213 32.455 1.00 37.27
45	ATOM	1753 C ARG 384 68.910 41.536 33.911 1.00 35.72
	ATOM	1754 O ARG 384 69.090 42.635 34.439 1.00 41.66
	ATOM	1755 N PHE 385 67.768 41.196 33.318 1.00 34.30
	ATOM	1756 CA PHE 385 66.646 42.119 33.199 1.00 32.40
	ATOM	1757 CB PHE 385 65.527 41.502 32.356 1.00 29.02
50	ATOM	1758 CG PHE 385 64.344 42.407 32.163 1.00 26.56

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ATOM 1759 CD1 PHE 385
                                64.317 43.320 31.119 1.00 26.59
    ATOM 1760 CD2 PHE 385
                                63,263 42,355 33,037 1,00 24,69
    ATOM 1761 CE1 PHE 385
                                63.231 44.173 30.947 1.00 31.70
    ATOM 1762 CE2 PHE 385
                                62.174 43.202 32.875 1.00 26.79
    ATOM 1763 CZ PHE 385
                               62.158 44.115 31.827 1.00 31.59
    ATOM 1764 C PHE 385
                               66.121 42.492 34.578 1.00 32.98
    ATOM 1765 O PHE 385
                               65.822 43.659 34.839 1.00 33.91
                               66.003 41.499 35.456 1.00 33.91
    ATOM 1766 N LEU 386
                                65.533 41.736 36.818 1.00 38.66
    ATOM 1767 CA LEU 386
    ATOM 1768 CB LEU 386
                                65.547 40.440 37.633 1.00 43.79
10
    ATOM 1769 CG LEU 386
                                64.327 39.521 37.525 1.00 49.81
    ATOM 1770 CD1 LEU 386
                                64.652 38.147 38.099 1.00 51.12
    ATOM 1771 CD2 LEU 386
                                63.135 40.148 38.246 1.00 49.17
                               66.445 42.761 37.475 1.00 38.95
    ATOM 1772 C LEU 386
    ATOM 1773 O LEU 386
                               65.979 43.682 38.146 1.00 42.16
15
    ATOM 1774 N HIS 387
                              67.745 42.613 37.248 1.00 33.62
                               68.723 43.531 37.808 1.00 39.73
    ATOM 1775 CA HIS 387
    ATOM 1776 CB HIS 387
                               70.138 42.980 37.639 1.00 40.71
    ATOM 1777 CG HIS 387
                               70.403 41.749 38.449 1.00 52.03
                                69.573 40.967 39.181 1.00 53.85
    ATOM 1778 CD2 HIS 387
20
                                71.657 41.189 38.566 1.00 54.79
    ATOM 1779 ND1 HIS 387
                                71.590 40.114 39.334 1.00 56.55
    ATOM 1780 CE1 HIS 387
    ATOM 1781 NE2 HIS 387
                                70.336 39.958 39.720 1.00 57.48
    ATOM 1782 C HIS 387
                              68.594 44.913 37.175 1.00 42.08
    ATOM 1783 O HIS 387
                              68.712 45.926 37.865 1.00 44.12
25
                               68.318 44.957 35.874 1.00 42.38
    ATOM 1784 N MET 388
                                68.154 46.229 35.175 1.00 38.00
    ATOM 1785 CA MET 388
    ATOM 1786 CB MET 388
                                67.840 46.006 33.692 1.00 40.21
    ATOM 1787 CG MET 388
                                69.009 45.555 32.829 1.00 41.26
    ATOM 1788 SD MET 388
                                68,500 45,427 31,089 1,00 45,51
30
    ATOM 1789 CE MET 388
                                69.089 43.802 30.645 1.00 42.40
    ATOM 1790 C MET 388
                               67.025 47.044 35.810 1.00 38.11
    ATOM 1791 O MET 388
                               67.155 48.255 35.997 1.00 38.41
    ATOM 1792 N LYS 389
                               65.926 46.374 36.144 1.00 39.67
                                64.773 47.036 36.750 1.00 44.96
35
    ATOM 1793 CA LYS 389
                                63.570 46.087 36.818 1.00 49.52
    ATOM 1794 CB LYS 389
    ATOM 1795 CG LYS 389
                                62.674 46.102 35.588 1.00 56.74
                                62.145 47.509 35.278 1.00 68.05
    ATOM 1796 CD LYS 389
    ATOM 1797 CE LYS 389
                                61.287 48.100 36.403 1.00 71.47
40
    ATOM 1798 NZ LYS 389
                                60.038 47.330 36.661 1.00 71.98
                               65.041 47.604 38.141 1.00 46.60
    ATOM 1799 C LYS 389
                               64.516 48.661 38.499 1.00 47.25
    ATOM 1800 O LYS 389
                               65.832 46.893 38.935 1.00 47.15
    ATOM 1801 N VAL 390
    ATOM 1802 CA VAL 390
                                66.129 47.353 40.284 1.00 50.75
    ATOM 1803 CB VAL 390
                                66,686 46,202 41,182 1,00 50,42
45
    ATOM 1804 CG1 VAL 390
                                68.095 45.802 40.770 1.00 47.93
                                66,650 46,612 42,640 1,00 56,67
    ATOM 1805 CG2 VAL 390
    ATOM 1806 C VAL 390
                               67.072 48.558 40.286 1.00 49.82
    ATOM 1807 O VAL 390
                               66.971 49.426 41.152 1.00 52.44
    ATOM 1808 N GLU 391
                               67.926 48.651 39.272 1.00 46.14
50
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	ATOM	1809 CA GLU 391	68.888 49.741 39.173 1.00 43.84
	ATOM	1810 CB GLU 391	70.150 49.268 38.449 1.00 41.44
	ATOM	1811 CG GLU 391	70.837 48.074 39.095 1.00 51.12
	ATOM	1812 CD GLU 391	71.218 48.325 40.540 1.00 57.29
5	ATOM	1813 OE1 GLU 391	71.970 49.287 40.802 1.00 58.15
	ATOM	1814 OE2 GLU 391	70.764 47.559 41.416 1.00 62.51
	ATOM	1815 C GLU 391	68.386 51.015 38.501 1.00 45.94
	ATOM	1816 O GLU 391	68.567 52.114 39.033 1.00 51.14
	ATOM	1817 N CYA 392	67.727 50.872 37.354 1.00 45.84
10	ATOM	1818 CA CYA 392	67.255 52.029 36.598 1.00 41.60
	ATOM	1819 CB CYA 392	67.681 51.889 35.140 1.00 42.06
	ATOM	1820 SG CYA 392	69.452 52.008 34.968 1.00 44.47
	ATOM	1821 AS CYA 392	69.867 50.812 33.150 1.00 54.22
	ATOM	1822 C CYA 392	65.779 52.395 36.683 1.00 42.27
15	ATOM	1823 O CYA 392	64.937 51.564 37.029 1.00 43.91
	ATOM	1824 N PRO 393	65.451 53.674 36.414 1.00 42.79
	ATOM	1825 CD PRO 393	66.384 54.774 36.106 1.00 38.59
	ATOM	1826 CA PRO 393	64.067 54.159 36.459 1.00 44.20
	ATOM	1827 CB PRO 393	64.218 55.667 36.238 1.00 39.88
20	ATOM	1828 CG PRO 393	65.487 55.789 35.459 1.00 35.88
	ATOM	1829 C PRO 393	63.178 53.513 35.398 1.00 45.29
	ATOM	1830 O PRO 393	63.600 53.308 34.257 1.00 43.97
	ATOM	1831 N THR 394	61.935 53.238 35.782 1.00 48.20
	ATOM	1832 CA THR 394	60.959 52.607 34.901 1.00 53.71
25	ATOM	1833 CB THR 394	59.605 52.429 35.629 1.00 59.59
	ATOM	1834 OG1 THR 394	58.690 51.717 34.787 1.00 66.50
	ATOM	1835 CG2 THR 394	59.013 53.787 36.004 1.00 61.00 60.752 53.358 33.581 1.00 51.35
	ATOM	1836 C THR 394	60.419 52.751 32.563 1.00 54.39
20	ATOM	1837 O THR 394 1838 N GLU 395	61.008 54.664 33.595 1.00 47.65
30	ATOM ATOM	1838 N GLU 395 1839 CA GLU 395	60.845 55.509 32.414 1.00 44.43
	ATOM	1840 CB GLU 395	60.988 56.978 32.804 1.00 43.85
	ATOM	1841 C GLU 395	61.788 55.175 31.250 1.00 42.93
	ATOM	1842 O GLU 395	61.589 55.649 30.129 1.00 41.39
35	ATOM	1843 N LEU 396	62.818 54.375 31.517 1.00 39.38
33	ATOM	1844 CA LEU 396	63.782 53.989 30.486 1.00 35.70
	ATOM	1845 CB LEU 396	65.185 53.867 31.090 1.00 34.96
	ATOM	1846 CG LEU 396	65,854 55,141 31,609 1,00 36,47
	ATOM	1847 CD1 LEU 396	67.234 54.807 32.150 1.00 34.21
40	ATOM	1848 CD2 LEU 396	65.959 56.164 30.491 1.00 32.74
-	ATOM	1849 C LEU 396	63.407 52.671 29.803 1.00 34.60
	ATOM	1850 O LEU 396	64.086 52.223 28.873 1.00 30.36
	ATOM	1851 N PHE 397	62.325 52.059 30.269 1.00 33.02
	ATOM	1852 CA PHE 397	61.868 50.792 29.725 1.00 33.39
45	ATOM	1853 CB PHE 397	61.615 49.782 30.852 1.00 34.30
	ATOM	1854 CG PHE 397	62.834 49.439 31.665 1.00 32.62
	ATOM	1855 CD1 PHE 397	63.296 50.301 32.654 1.00 32.35
	ATOM	1856 CD2 PHE 397	63.504 48.241 31.461 1.00 31.28
	ATOM	1857 CE1 PHE 397	64.407 49.976 33.426 1.00 27.01
50	ATOM	1858 CE2 PHE 397	64.616 47.905 32.229 1.00 33.34

	ATOM	1859 CZ PHE 397	65.067 48.775 33.213 1.00 31.29
		1860 C PHE 397	60.580 50.961 28.934 1.00 33.17
	ATOM		59.540 51.318 29.498 1.00 31.99
	ATOM		60.636 50.752 27.606 1.00 32.45
_	ATOM		61.821 50.493 26.768 1.00 28.15
5	ATOM	1863 CD PRO 398	59.429 50.885 26.786 1.00 30.02
	ATOM	1864 CA PRO 398	59,921 50.483 25.394 1.00 38.15
	ATOM	1865 CB PRO 398	
	ATOM	1866 CG PRO 398	61.352 50.923 25.397 1.00 24.89
	ATOM	1867 C PRO 398	58.384 49.900 27.326 1.00 28.39
10	ATOM	1868 O PRO 398	58.735 48.810 27.789 1.00 28.00
	ATOM	1869 N PRO 399	57.092 50.262 27.267 1.00 32.45
	ATOM	1870 CD PRO 399	56.577 51.511 26.672 1.00 34.93
	ATOM	1871 CA PRO 399	55.989 49.421 27.753 1.00 32.54
	ATOM	1872 CB PRO 399	54.755 50.122 27.188 1.00 34.47
15	ATOM	1873 CG PRO 399	55.159 51.564 27.196 1.00 31.37
	ATOM	1874 C PRO 399	56.044 47.946 27.338 1.00 32.18
	ATOM	1875 O PRO 399	55.950 47.054 28.188 1.00 32.58
	ATOM	1876 N LEU 400	56.195 47.689 26.041 1.00 30.15
	ATOM	1877 CA LEU 400	56.259 46.314 25.541 1.00 32.32
20	ATOM	1878 CB LEU 400	56.211 46.297 24.011 1.00 28.67
	ATOM	1879 CG LEU 400	56.028 44.927 23.351 1.00 28.77
	ATOM	1880 CD1 LEU 400	54.802 44.234 23.919 1.00 22.73
	ATOM	1881 CD2 LEU 400	55.897 45.096 21.846 1.00 27.89
	ATOM	1882 C LEU 400	57.496 45.561 26.051 1.00 32.27
25	ATOM	1883 O LEU 400	57.437 44.358 26.307 1.00 32.87
	ATOM	1884 N PHE 401	58.602 46.279 26.215 1.00 32.27
	ATOM	1885 CA PHE 401	59.847 45.695 26.710 1.00 32.39
	ATOM	1886 CB PHE 401	60.946 46.769 26.711 1.00 31.38
	ATOM	1887 CG PHE 401	62.290 46.286 27.194 1.00 35.12
30	ATOM	1888 CD1 PHE 401	62.835 45.089 26.729 1.00 34.68
	ATOM	1889 CD2 PHE 401	63.030 47.051 28.097 1.00 34.57
	ATOM	1890 CE1 PHE 401	64.100 44.662 27.155 1.00 30.27
	ATOM	1891 CE2 PHE 401	64.291 46.635 28.526 1.00 33.57
	ATOM	1892 CZ PHE 401	64.828 45.438 28.054 1.00 35.74
35	ATOM	1893 C PHE 401	59.599 45.169 28.129 1.00 32.21
	ATOM	1894 O PHE 401	60.002 44.056 28.478 1.00 33.36
	ATOM	1895 N LEU 402	58.902 45.967 28.929 1.00 31.85
	ATOM	1896 CA LEU 402	58.582 45.602 30.302 1.00 35.06
	ATOM	1897 CB LEU 402	57.948 46.789 31.029 1.00 34.76
40	ATOM	1898 CG LEU 402	58.878 47.852 31.591 1.00 33.48
	ATOM	1899 CD1 LEU 402	58.060 49.010 32.152 1.00 32.58
	ATOM	1900 CD2 LEU 402	59.753 47.217 32.662 1.00 26.27
	ATOM	1901 C LEU 402	57.626 44.426 30.393 1.00 36.80
	ATOM	1902 O LEU 402	57.793 43.545 31.239 1.00 35.43
45	ATOM	1903 N GLU 403	56.600 44.443 29.547 1.00 38.50
	ATOM	1904 CA GLU 403	55.581 43.401 29.540 1.00 40.24
	ATOM	1905 CB GLU 403	54.435 43.792 28.605 1.00 44.03
	ATOM	1906 CG GLU 403	53.239 42.850 28.666 1.00 55.53
	ATOM	1907 CD GLU 403	52.180 43.159 27.618 1.00 66.67
50	ATOM	1908 OE1 GLU 403	52.151 44.299 27.095 1.00 70.81

	ATOM	1909 OE2 GLU 403	51.370 42.255 27.315 1.00 73.80
	ATOM	1910 C GLU 403	56.096 42.018 29.162 1.00 38.00
	ATOM	1911 O GLU 403	55.745 41.029 29.805 1.00 38.78
	ATOM	1912 N VAL 404	56.934 41.955 28.132 1.00 37.39
5	ATOM	1913 CA VAL 404	57.475 40.686 27.652 1.00 37.05
-	ATOM	1914 CB VAL 404	58.180 40.855 26.286 1.00 35.57
	ATOM	1915 CG1 VAL 404	58.677 39.513 25.776 1.00 36.85
	ATOM	1916 CG2 VAL 404	57.222 41.451 25.287 1.00 42.03
	ATOM	1917 C VAL 404	58.438 40.000 28.609 1.00 38.69
10	ATOM	1918 O VAL 404	58.436 38.774 28.727 1.00 40.71
	ATOM	1919 N PHE 405	59.267 40.785 29.286 1.00 39.34
	ATOM	1920 CA PHE 405	60.250 40.221 30.198 1.00 39.33
	ATOM	1921 CB PHE 405	61.620 40.840 29.913 1.00 33.87
	ATOM	1922 CG PHE 405	62.107 40.609 28.509 1.00 32.17
15	ATOM	1923 CD1 PHE 405	62.355 41.683 27.660 1.00 31.34
	ATOM	1924 CD2 PHE 405	62.315 39.317 28.032 1.00 31.98
	ATOM	1925 CE1 PHE 405	62.801 41.476 26.352 1.00 30.79
	ATOM	1926 CE2 PHE 405	62.759 39.099 26.730 1.00 26.06
	ATOM	1927 CZ PHE 405	63.004 40.182 25.889 1.00 27.98
20	ATOM	1928 C PHE 405	59.905 40.322 31.682 1.00 42.64
	ATOM	1929 O PHE 405	60.785 40.188 32.534 1.00 45.10
	ATOM	1930 N GLU 406	58.630 40.536 31.988 1.00 48.95
	ATOM	1931 CA GLU 406	58.181 40.641 33.373 1.00 56.93
	ATOM	1932 CB GLU 406	56.820 41.324 33.432 1.00 56.94
25	ATOM	1933 C GLU 406	58.116 39.263 34.040 1.00 61.92
	ATOM	1934 O GLU 406	57.988 38.256 33.308 1.00 67.61
	ATOM	1 O1 HOH 501	67.588 36.828 11.225 1.00 27.32
	ATOM	2 O1 HOH 502	68.647 41.203 12.940 1.00 39.54
	ATOM	3 O1 HOH 503	64.072 40.115 12.407 1.00 32.47
30	ATOM	4 O1 HOH 504	62.312 39.659 16.075 1.00 17.39
	ATOM	5 O1 HOH 505	63.449 46.468 15.530 1.00 30.46
	ATOM	6 O1 HOH 506	67.191 15.561 -0.279 1.00 35.96 67.100 11.855 0.295 1.00 20.00
	ATOM	7 O1 HOH 507	
	ATOM	8 O1 HOH 508	
35	ATOM	9 O1 HOH 509	59.851 10.761 6.050 1.00 20.00 57.553 11.824 10.360 1.00 44.63
	ATOM	10 O1 HOH 510	
	ATOM	11 O1 HOH 511	54.101 13.545 8.720 1.00 20.00 55.923 15.916 12.205 1.00 29.31
	ATOM	12 O1 HOH 512 13 O1 HOH 513	50,900 19.934 8.193 1.00 20.00
40	ATOM		50.474 22.912 7.942 1.00 45.34
40	ATOM	14 O1 HOH 514 15 O1 HOH 515	49,737 20.631 11.530 1.00 20.00
	ATOM ATOM	15 O1 HOH 515 16 O1 HOH 516	50.829 25.467 13.330 1.00 20.00
	ATOM	17 O1 HOH 517	53.818 25.833 10.682 1.00 42.12
	ATOM	18 O1 HOH 518	52.591 31.216 7.313 1.00 35.55
45	ATOM	19 O1 HOH 519	58.510 31.667 2.158 1.00 20.00
43	ATOM	20 O1 HOH 520	58.235 36.751 2.232 1.00 20.00
	ATOM		62.484 37.992 5.537 1.00 20.00
	ATOM	22 O1 HOH 522	68.184 36.969 5.889 1.00 50.08
	ATOM		66.889 33.781 8.584 1.00 20.00
50	ATOM		67.217 30.836 3.085 1.00 34.44
			

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	4.000.4	06 01 11011	E26	64.336 28.325 3.098 1.00 20.00
	ATOM	25 O1 HOH	525	
	ATOM	26 O1 HOH	526	67.667 26.625 1.519 1.00 20.00
	ATOM	27 O1 HOH	527	76.757 22.883 5.467 1.00 36.94
	ATOM	28 O1 HOH	528	72.250 17.936 6.950 1.00 36.00
5	ATOM	29 O1 HOH	529	71.760 14.791 8.058 1.00 40.18
	ATOM	30 O1 HOH	530	72.884 14.751 11.484 1.00 41.44
	ATOM	31 O1 HOH	531	69.235 12.986 11.709 1.00 39.38
	ATOM	32 O1 HOH	532	69.402 12.036 14.891 1.00 40.68
	ATOM	33 O1 HOH	533	64.560 10.910 15.076 1.00 20.00
10	ATOM	34 O1 HOH	534	63.169 10.413 11.722 1.00 20.00
••	ATOM	35 O1 HOH	535	66.042 11.455 11.077 1.00 41.05
	ATOM	36 O1 HOH	536	76,285 12.458 10.677 1.00 20.00
	ATOM	37 O1 HOH	537	81.094 22.520 13.435 1.00 48.70
	ATOM	38 O1 HOH	538	80.505 25.457 14.849 1.00 46.30
15	ATOM	39 O1 HOH	539	77.669 21.932 18.119 1.00 43.79
15	ATOM	40 O1 HOH	540	77.187 28.903 21.137 1.00 40.22
	ATOM	41 O1 HOH	541	76.420 30.760 23.658 1.00 29.63
		42 O1 HOH	542	83.028 32.743 20.922 1.00 38.14
	ATOM	43 O1 HOH	543	82.842 43.133 17.983 1.00 39.36
20	ATOM		544	77.484 34.040 9.664 1.00 36.37
20	ATOM			75.904 32.986 12.256 1.00 34.93
	ATOM	45 O1 HOH	545	
	ATOM	46 O1 HOH	546	
	ATOM	47 O1 HOH	547	
	ATOM	48 O1 HOH	548	
25	ATOM	49 O1 HOH	549	59.544 21.463 26.162 1.00 20.00
	ATOM	50 O1 HOH	550	62.300 27.528 24.386 1.00 35.89
	ATOM	51 O1 HOH	551	58.228 29.424 24.603 1.00 25.47
	ATOM	52 O1 HOH	552	57.368 32.196 30.527 1.00 45.27
	ATOM	53 O1 HOH	553	62.063 36.304 30.245 1.00 42.26
30	ATOM	54 O1 HOH	554	64.722 36.725 28.906 1.00 24.66
	ATOM	55 O1 HOH	555	62.207 35.851 26.642 1.00 30.36
	ATOM	56 O1 HOH	556	63.608 33.715 25.707 1.00 42.74
	ATOM	57 O1 HOH	557	62.979 38.422 32.977 1.00 49.93
	ATOM	58 O1 HOH	558	66.911 33.364 34.901 1.00 50.02
35	ATOM	59 O1 HOH	559	72.608 29.636 31.674 1.00 37.60
	ATOM	60 O1 HOH	560	76.967 40.633 32.514 1.00 44.81
	ATOM	61 O1 HOH	561	73.613 41.817 36.847 1.00 31.79
	ATOM	62 O1 HOH	562	75.773 46.227 30.514 1.00 29.06
	ATOM	63 O1 HOH	563	79.903 46.178 30.800 1.00 41.67
40	ATOM	64 O1 HOH	564	69.746 51.175 33.564 1.00 20.00
	ATOM	65 O1 HOH	565	74.320 52.047 39.438 1.00 20.00
	ATOM	66 O1 HOH	566	65.900 53.647 27.404 1.00 40.45
	ATOM	67 O1 HOH	567	68.848 53.076 17.895 1.00 39.25
	ATOM	68 O1 HOH	568	63.507 48.672 13.581 1.00 43.77
45	ATOM	69 O1 HOH	569	64.625 46.825 10.331 1.00 20.00
73	ATOM	70 O1 HOH	570	55.882 41.431 11.148 1.00 20.00
	ATOM	71 O1 HOH	571	52.830 43.513 20.032 1.00 35.18
		71 O1 HOH 72 O1 HOH	572	56.990 49.485 24.052 1.00 37.30
	ATOM		573	54.188 47.024 30.900 1.00 52.93
50	ATOM			57.823 44.590 34.025 1.00 53.64
50	ATOM	74 O1 HOH	574	37.023 44.370 34.023 1.00 33.04

	ATOM	75 O1 HOH 575	47.827 29.597 30.690 1.00 37.61
	ATOM	76 O1 HOH 576	53.030 24.901 32.732 1.00 45.06
	ATOM	77 O1 HOH 577	47.569 19.105 28.647 1.00 38.88
	ATOM	78 O1 HOH 578	47.232 20.282 25.561 1.00 20.00
5	ATOM	79 O1 HOH 579	51.960 14.869 25.534 1.00 49.45
ر	ATOM	80 O1 HOH 580	52.831 23.395 1.634 1.00 20.00
	ATOM	81 O1 HOH 581	51.472 22.968 -0.900 1.00 25.10
	ATOM	82 O1 HOH 582	77.238 52.503 8.906 1.00 47.05
	END	02 01 11011 302	77.230 32,303 0,500 2000 1.00
10	ATOM	2004 C1 DMT 1	67.320 42.326 18.648 1.00 28.58
	ATOM	2005 C2 DMT 1	68.927 43.263 23.318 1.00 29.26
	ATOM	2006 C3 DMT 1	67.236 43.583 19.236 1.00 24.54
	ATOM	2007 C4 DMT 1	69.268 44.313 24.111 1.00 28.48
	ATOM	2008 C5 DMT 1	68.003 43.859 20.363 1.00 28.76
15	ATOM	2009 C6 DMT 1	68.654 44.389 25.458 1.00 28.16
	ATOM	2010 C7 DMT 1	68.811 42.902 20.875 1.00 26.80
	ATOM	2011 C8 DMT 1	67.803 43.410 25.793 1.00 29.83
	ATOM	2012 C9 DMT 1	68.921 41.665 20.324 1.00 26.77
	ATOM	2013 C10 DMT 1	67.464 42.358 24.989 1.00 28.60
20	ATOM	2014 C11 DMT 1	68.165 41.349 19.185 1.00 25.29
	ATOM	2015 C12 DMT 1	68.059 42.281 23.675 1.00 26.74
	ATOM	2016 C13 DMT 1	66.475 42.038 17.456 1.00 21.51
	ATOM	2017 C14 DMT 1	68.916 45.478 26.380 1.00 21.05
	ATOM	2018 C15 DMT 1	66.989 40.910 16.417 1.00 22.84
25	ATOM	2019 C16 DMT 1	68.090 46.870 26.009 1.00 19.41
	ATOM	2020 C17 DMT 1	65.982 40.730 15.243 1.00 27.07
	ATOM	2021 C18 DMT 1	70.279 46.131 26.085 1.00 16.03
	ATOM	2022 C19 DMT 1	67.903 45.249 20.974 1.00 19.56
	ATOM	2023 C20 DMT 1	69.853 40.599 20.901 1.00 4.52
30	ATOM	2024 N1 DMT 1	68.280 41.070 16.042 1.00 17.57
	ATOM	2025 O1 DMT 1	67.209 43.465 27.087 1.00 25.94
	ATOM	2026 O2 DMT 1	69.547 43.191 22.015 1.00 30.23
	ATOM	2027 O3 DMT 1	66.449 40.778 14.118 1.00 29.45
	ATOM	2028 O4 DMT 1	64.820 40.564 15.546 1.00 26.46
35	END		

PCT/US98/25296 WO 99/26966

APPENDIX 4

TR TRIAC.PDB

REMARK

REMARK TR triac full length numbering

REMARK Rfactor 0.236 Rfree 0.241

REMARK Resolution 25. 2.5 all reflections

REMARK

REMARK Three cacodylate-modified cysteines:

REMARK Cys334, Cys380, Cys392

REMARK modeled as free arsenic atoms 10

REMARK

REMARK conserved polar HOH numbered as in TR_t3.pdb

REMARK rearrangements start 600

REMARK side chain of certain residues modeled as ALA due to poor density; 15

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al. 20

REMARK in the following codons:

REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409 25

M.B. MURRAY, N.D.ZILZ, **AUTH JRNL**

N.L.MCCREARY, M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA **JRNL**

CLONES FOR TWO 30

TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL

JRNL REF JBC

V. 263 25 1988 AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS

V. 237 1987

JRNL IDENTIFICATION OF A NOVEL THYROID HORMONE JRNL

RECEPTOR EXPRESSED 35

TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM JRNL

REF SCIENCE JRNL

AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM **JRNL**

TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED JRNL

40 BY ALTERNATIVE

ATOM

45

TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR JRNL

GENE TRANSCRIPT REF NUC. ACIDS. RES. V. 16 12 1988 JRNL

REMARK

9.880 -24.199 7.196 1.00 57.79 1 CB ARG 157

11.380 -24.411 7.340 1.00 57.79 ATOM 2 CG ARG 157

11.960 -23.602 8.486 1.00 57.79 3 CD ARG 157 ATOM

11.492 -24.098 9.778 1.00 57.79 ATOM 4 NE ARG 157

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12.284 -24.379 10.809 1.00 57.79
              5 CZ ARG 157
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             6 NH1 ARG 157
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                                11.762 -24.854 11.932 1.00 57.79
             7 NH2 ARG 157
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                               7.774 -24.838 5.974 1.00 38.50
             8 C ARG 157
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             9 O ARG 157
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                                6.945 -25.424 8.282 1.00 28.38
             13 CD PRO 158
    ATOM
                                5.415 -24.562 6.617 1.00 23.08
             14 CA PRO 158
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             16 CG PRO 158
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             20 CA GLU 159
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             31 CB PRO 160
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             36 CA THR 161
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              54 OE1 GLU 163
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              83 CB ASP 166
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     ATOM
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              85 OD1 ASP 166
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              93 CD1 LEU 167
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              94 CD2 LEU 167
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     ATOM
              98 CA ILE 168
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              99 CB ILE 168
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             100 CG2 ILE 168
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             103 C ILE 168
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             104 O ILE 168
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	ATOM	106 CA HIS 169	-2.342 -8.674 4.245 1.00 12.99
	ATOM	107 CB HIS 169	-3.218 -9.087 3.062 1.00 13.09
	ATOM	108 CG HIS 169	-2.553 -10.045 2.126 1.00 13.09
5	ATOM	109 CD2 HIS 169	-1.247 -10.223 1.811 1.00 13.09
-	ATOM	110 ND1 HIS 169	-3.249 -11.000 1.416 1.00 13.09
	ATOM	111 CE1 HIS 169	-2.403 -11.728 0.710 1.00 13.09
	ATOM	112 NE2 HIS 169	-1.181 -11.277 0.936 1.00 13.09
	ATOM	113 C HIS 169	-3.017 -7.550 5.017 1.00 12.99
10	ATOM	114 O HIS 169	-2.680 -6.377 4.839 1.00 13.09
	ATOM	115 N VAL 170	-3.978 -7.909 5.862 1.00 13.36
	ATOM	116 CA VAL 170	-4.696 -6.926 6.664 1.00 13.36
	ATOM	117 CB VAL 170	-5.863 -7.572 7.443 1.00 20.12
	ATOM	118 CG1 VAL 170	-6.541 -6.540 8.340 1.00 20.12
15	ATOM	119 CG2 VAL 170	-6.869 -8.165 6.471 1.00 20.12
	ATOM	120 C VAL 170	-3.741 -6.246 7.639 1.00 13.36
	ATOM	121 O VAL 170	-3.728 -5.019 7.744 1.00 20.12
	ATOM	122 N ALA 171	-2.920 -7.043 8.320 1.00 11.04
	ATOM	123 CA ALA 171	-1.953 -6.515 9.277 1.00 11.04
20	ATOM	124 CB ALA 171	-1.249 -7.653 10.005 1.00 13.43
	ATOM	125 C ALA 171	-0.931 -5.613 8.588 1.00 11.04
	ATOM	126 O ALA 171	-0.658 -4.507 9.058 1.00 13.43
	ATOM	127 N THR 172	-0.382 -6.076 7.469 1.00 12.51
	ATOM	128 CA THR 172	0.606 -5.301 6.723 1.00 12.51
25	ATOM	129 CB THR 172	1.062 -6.032 5.445 1.00 14.17
	ATOM	130 OG1 THR 172	1.548 -7.338 5.782 1.00 14.17
	ATOM	131 CG2 THR 172	2.175 -5.255 4.756 1.00 14.17
	ATOM	132 C THR 172	0.045 -3.936 6.337 1.00 12.51
	ATOM	133 O THR 172	0.701 -2.910 6.537 1.00 14.17
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	ATOM	135 CA GLU 173	-1.818 -2.675 5.421 1.00 17.79 -3.130 -2.946 4.682 1.00 49.44
	ATOM	136 CB GLU 173	
	ATOM	137 CG GLU 173	-3.823 -1.679 4.171 1.00 49.44 -2.930 -0.835 3.266 1.00 49.44
2.5	ATOM	138 CD GLU 173	-2.930 -0.833 3.266 1.00 49.44
35	ATOM	139 OE1 GLU 173 140 OE2 GLU 173	-3.085 0.404 3.269 1.00 49.44
	ATOM		-2.072 -1.780 6.628 1.00 17.79
	ATOM	141 C GLU 173 142 O GLU 173	-1.854 -0.568 6.557 1.00 49.44
	ATOM	142 U GLU 173 143 N ALA 174	-2.525 -2.375 7.731 1.00 13.12
40	ATOM	143 N ALA 174 144 CA ALA 174	
40	ATOM ATOM	145 CB ALA 174	-3.226 -2.576 10.068 1.00 17.51
	ATOM	145 CB ALA 174	-1.556 -0.856 9.375 1.00 13.12
	ATOM	147 O ALA 174	-1.634 0.319 9.735 1.00 17.51
	ATOM	148 N HIS 175	-0.409 -1.521 9.317 1.00 12.20
45	ATOM	149 CA HIS 175	0.851 -0.895 9.679 1.00 12.20
73	ATOM	150 CB HIS 175	1.944 -1.949 9.886 1.00 17.52
	ATOM	150 CB HIS 175	3.302 -1.365 10.136 1.00 17.52
	ATOM	151 CO HIS 175	3.733 -0.468 11.055 1.00 17.52
	ATOM	153 ND1 HIS 175	4.400 -1.679 9.364 1.00 17.52
50	ATOM	154 CE1 HIS 175	5.447 -0.999 9.793 1.00 17.52
-		-3	• •

ATOM 156 C HIS 175 ATOM 157 O HIS 175 ATOM 158 N ARG 176 ATOM 158 N ARG 176 ATOM 159 CA ARG 176 ATOM 160 CB ARG 176 ATOM 161 CG ARG 176 ATOM 161 CG ARG 176 ATOM 162 CD ARG 176 ATOM 163 NE ARG 176 ATOM 163 NE ARG 176 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 178 OG1 THR 178 ATOM 179 CG2 THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 185 CG ASN 179 ATOM 187 ND2 ASN 179 ATOM 187 ND2 ASN 179 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 194 C ALA 181 ATOM 195 CR ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 198 C ALA 18				
ATOM 157 O HIS 175 ATOM 158 N ARG 176 ATOM 159 CA ARG 176 ATOM 160 CB ARG 176 ATOM 161 CG ARG 176 ATOM 161 CG ARG 176 ATOM 162 CD ARG 176 ATOM 163 NE ARG 176 ATOM 163 NE ARG 176 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 185 CG ASN 179 ATOM 186 CA ALA 180 ATOM 194 CA ALA 180 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 199 O ALA 181 ATOM 190 O ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 199 O ALA 181 ATOM 190 O ALA 181 ATOM 190 O ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 200 N GLY 182 ATOM 201 CG CLY 182 ATOM 202 C GLY 182 ATOM 203 O GLY 182		ATOM		5.070 -0.258 10.818 1.00 17.52
ATOM 158 N ARG 176 ATOM 159 CA ARG 176 ATOM 160 CB ARG 176 ATOM 161 CG ARG 176 ATOM 161 CG ARG 176 ATOM 162 CD ARG 176 ATOM 162 CD ARG 176 ATOM 163 NE ARG 176 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 N ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 173 C SER 177 ATOM 174 O SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 178 OG1 THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 187 ND2 ASN 179 ATOM 187 ND2 ASN 179 ATOM 187 ND2 ASN 179 ATOM 188 C ASN 179 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 195 C ALA 180 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 191 CA ALA 181 ATOM 195 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 O RIA 181 ATOM 190 O ALA 181 ATOM 190 C ALA 181 ATOM 190 O ALA 181 ATOM 201 CA GLY 182 ATOM 202 C GLY 182 ATOM 203 O GLY 182 ATOM 204 0 AGN 182 ATOM 203 O GLY 182 ATOM 203 O GLY 182		ATOM	- -	
5 ATOM 159 CA ARG 176 ATOM 160 CB ARG 176 ATOM 161 CG ARG 176 ATOM 161 CG ARG 176 ATOM 162 CD ARG 176 ATOM 163 NE ARG 176 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 173 C SER 177 ATOM 174 O SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 176 CA THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 185 CG ASN 179 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 190 N GLY 182 ATOM 202 C GLY 182 ATOM 203 O GLY 182 ATOM 203 O GLY 182 ATOM 204 A.485 1.0034.		ATOM	157 O HIS 175	
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ATOM 163 NE ARG 176 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 173 C SER 177 ATOM 174 O SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 178 OG1 THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 185 CG ASN 179 ATOM 189 O ASN 179 ATOM 189 O ASN 179 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 193 C ALA 180 ATOM 194 O ALA 180 ATOM 195 N ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 191 CB ALA 181 ATOM 192 CB ALA 181 ATOM 194 O ALA 181 ATOM 195 C ALA 181 ATOM 196 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N GLY 182 ATOM 190 C GLY 182 ATOM 190 C GLY 182 ATOM 190 ALA 181 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 193 C ALA 181 ATOM 194 O ALA 181 ATOM 195 N ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 191 CA ALA 181 ATOM 192 CB ALA 181 ATOM 193 C ALA 181 ATOM 194 O ALA 181 ATOM 195 N ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 191 CA ALA 181 ATOM 192 CB ALA 181 ATOM 193 C ALA 181 ATOM 194 O ALA 181 ATOM 195 N ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 190		ATOM	161 CG ARG 176	2.683 -1.088 4.730 1.00 50.41
10 ATOM 164 CZ ARG 176 ATOM 165 NH1 ARG 176 ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 173 C SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 178 OG1 THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 185 CG ASN 179 ATOM 186 OASN 179 ATOM 187 CB ALA 180 ATOM 189 O ASN 179 ATOM 180 C ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 180 ATOM 193 C ALA 180 ATOM 194 O ALA 180 ATOM 195 CA ALA 181 ATOM 197 CB ALA 181 ATOM 190 N ALA 180 ATOM 191 CB ALA 181 ATOM 192 CB ALA 181 ATOM 195 CA GLY 182 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 190 N ALA 181 ATOM 190 C ALA 181 ATOM 190 C ALA 181 ATOM 190 C ALA 181 ATOM 202 C GLY 182 ATOM 203 O GLY 182		ATOM	162 CD ARG 176	2.666 -1.565 3.299 1.00 50.41
ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 CG SER 177 ATOM 173 C SER 177 ATOM 174 O SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 185 CG ASN 179 ATOM 186 C ALA 180 ATOM 187 O SALA 180 ATOM 189 O ASN 179 ATOM 180 C ALA 180 ATOM 181 O ALA 180 ATOM 192 CB ALA 180 ATOM 193 C ALA 181 ATOM 194 O ALA 180 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 180 ATOM 197 CB ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 200 C GLY 182 ATOM 200 C		ATOM	163 NE ARG 176	3.682 -2.571 2.989 1.00 50.41
ATOM 165 NH1 ARG 176 ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 173 C SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 O THR 178 ATOM 182 N ASN 179 ATOM 183 CA ASN 179 ATOM 184 CB ASN 179 ATOM 185 C ASN 179 ATOM 186 OASN 179 ATOM 187 OASN 179 ATOM 187 CB ALA 180 ATOM 189 O ASN 179 ATOM 180 C ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 180 ATOM 194 O ALA 180 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 199 O ALA 181 ATOM 190 C AGLY 182 ATOM 190 C AGLY 182 ATOM 190 C AGLY 182 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 198 C ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 194 C ALA 181 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 181 ATOM 190 N ALA 181 ATOM 190 C ALA 181 ATOM 191 CA ALA 181 ATOM 192 CB ALA 181 ATOM 194 C ALA 181 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 O ALA 181 ATOM 190 N ALA 180 ATOM 190 N ALA 181 ATOM 190 C ALA 181 ATOM 202 C GLY 182 ATOM 203 O GLY 182	10	ATOM	164 CZ ARG 176	3.577 -3.472 2.012 1.00 50.41
ATOM 166 NH2 ARG 176 ATOM 167 C ARG 176 ATOM 168 O ARG 176 ATOM 169 N SER 177 ATOM 170 CA SER 177 ATOM 171 CB SER 177 ATOM 172 OG SER 177 ATOM 173 C SER 177 ATOM 175 N THR 178 ATOM 176 CA THR 178 ATOM 177 CB THR 178 ATOM 179 CG2 THR 178 ATOM 180 C THR 178 ATOM 181 O THR 178 ATOM 181 CB ASN 179 ATOM 184 CB ASN 179 ATOM 185 CG ASN 179 ATOM 186 OD1 ASN 179 ATOM 186 CA ALA 180 ATOM 191 CA ALA 180 ATOM 192 CB ALA 181 ATOM 196 CA ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 C ALA 181 ATOM 190 N ALA 180 ATOM 190 C ALA 181 ATOM 191 CA GLY 182 ATOM 190 C GLY 182 ATOM 190 C ALA 181 ATOM 191 CA ALA 181 ATOM 192 CB ALA 181 ATOM 195 C ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 C ALA 181 ATOM 190 C GLY 182 ATOM 190 C GLY 182 ATOM 190 C ALA 181 ATOM 191 CA ALA 181 ATOM 192 CB ALA 181 ATOM 194 CA ALA 181 ATOM 195 CA ALA 181 ATOM 196 CA ALA 181 ATOM 197 CB ALA 181 ATOM 198 C ALA 181 ATOM 199 CA ALA 181 ATOM 190 CA GLY 182 ATOM 200 C GLY 182 ATOM 201 CA GLY 182 ATOM 201 CA GLY 182 ATOM 202 C GLY 182 ATOM 203 C GLY 182 ATOM 203 C GLY 182 ATOM 204 A-785 5.334 1.00 48.5		ATOM	165 NH1 ARG 176	2.496 -3.513 1.236 1.00 50.41
ATOM 167 C ARG 176			166 NH2 ARG 176	4.536 -4.376 1.841 1.00 50.41
ATOM 168 O ARG 176				0.972 1.988 6.306 1.00 12.54
15 ATOM 169 N SER 177 -0.326 1.935 6.581 1.00 24.74 ATOM 170 CA SER 177 -1.147 3.145 6.584 1.00 24.74 ATOM 171 CB SER 177 -2.622 2.792 6.414 1.00 21.5 ATOM 172 OG SER 177 -3.069 1.913 7.436 1.00 21.5 ATOM 173 C SER 177 -0.960 4.013 7.832 1.00 24.72 20 ATOM 174 O SER 177 -1.401 5.159 7.863 1.00 21.5 ATOM 175 N THR 178 -0.347 3.453 8.870 1.00 17.9 ATOM 176 CA THR 178 -0.347 3.453 8.870 1.00 17.9 ATOM 177 CB THR 178 -0.347 3.453 8.870 1.00 17.9 ATOM 178 OG1 THR 178 -0.265 2.091 11.361 1.00 19.7 ATOM 180 C THR 178 -2.253 3.443 11.211 1.00 19.7 ATOM 181 O THR 178 1.376 4.395 10.382 1.00 17.9 ATOM 181 O THR 178 1.376 4.395 10.382 1.00 17.9 ATOM 182 N ASN 179 2.207 4.024 9.417 1.00 25.8 ATOM 184 CB ASN 179 3.654 4.180 9.546 1.00 25.8 ATOM 185 CG ASN 179 4.362 2.974 8.943 1.00 44.2 ATOM 186 OD1 ASN 179 6.719 2.830 8.391 1.00 44.2 ATOM 188 C ASN 179 6.719 2.830 8.391 1.00 44.2 ATOM 190 N ALA 180 4.332 6.502 9.604 1.00 45.2 ATOM 191 CA ALA 180 4.740 7.818 9.126 1.00 45.2 ATOM 194 O ALA 180 6.918 7.097 8.372 1.00 36.1 ATOM 195 N ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 O ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 C ALA 181 8.170 9.116 6.722 1.00 50. ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 C ALA 181 7.069 7.427 5.196 1.00 39.0 ATOM 201 CA GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 202 C GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5				1.561 3.040 6.087 1.00 50.41
ATOM 170 CA SER 177 -1.147 3.145 6.584 1.00 24.7 ATOM 171 CB SER 177 -2.622 2.792 6.414 1.00 21.5 ATOM 172 OG SER 177 -3.069 1.913 7.436 1.00 21.5 ATOM 173 C SER 177 -0.960 4.013 7.832 1.00 24.7 20 ATOM 174 O SER 177 -1.401 5.159 7.863 1.00 21.5 ATOM 175 N THR 178 -0.347 3.453 8.870 1.00 17.9 ATOM 176 CA THR 178 -0.104 4.181 10.115 1.00 17.9 ATOM 177 CB THR 178 -0.265 2.091 11.361 1.00 19. ATOM 179 CG2 THR 178 -0.265 2.091 11.361 1.00 19. ATOM 180 C THR 178 -0.265 2.091 11.361 1.00 19. ATOM 181 O THR 178 1.376 4.395 10.382 1.00 17.9 ATOM 181 O THR 178 1.366 4.395 10.382 1.00 17.9 ATOM 182 N ASN 179 2.207 4.024 9.417 1.00 25.8 ATOM 183 CA ASN 179 3.654 4.180 9.546 1.00 25.8 ATOM 184 CB ASN 179 4.362 2.974 8.943 1.00 44.2 ATOM 185 CG ASN 179 5.817 2.871 9.368 1.00 44.2 ATOM 186 OD1 ASN 179 6.129 2.768 10.564 1.00 44.2 ATOM 187 ND2 ASN 179 6.129 2.768 10.564 1.00 44.2 ATOM 188 C ASN 179 4.078 5.458 8.823 1.00 25.8 ATOM 190 N ALA 180 4.332 6.502 9.604 1.00 45.2 ATOM 191 CA ALA 180 4.740 7.818 9.126 1.00 45.2 ATOM 193 C ALA 180 5.026 8.743 10.313 1.00 36.1 ATOM 194 O ALA 180 6.918 7.097 8.372 1.00 36.1 ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 201 CA GLY 182 6.676 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 6.676 5.040 4.867 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5	15			-0.326 1.935 6.581 1.00 24.74
ATOM 171 CB SER 177 -2.622 2.792 6.414 1.00 21.5 ATOM 172 OG SER 177 -3.069 1.913 7.436 1.00 21.5 ATOM 173 C SER 177 -0.960 4.013 7.832 1.00 24.74 20 ATOM 174 O SER 177 -1.401 5.159 7.863 1.00 21.5 ATOM 175 N THR 178 -0.347 3.453 8.870 1.00 17.9 ATOM 176 CA THR 178 -0.104 4.181 10.115 1.00 17. ATOM 177 CB THR 178 -0.736 3.440 11.323 1.00 19. ATOM 179 CG2 THR 178 -0.265 2.091 11.361 1.00 19. ATOM 180 C THR 178 1.376 4.395 10.382 1.00 17.9 ATOM 181 O THR 178 1.376 4.395 10.382 1.00 17.9 ATOM 182 N ASN 179 2.207 4.024 9.417 1.00 25.3 ATOM 183 CA ASN 179 3.654 4.180 9.546 1.00 25.3 ATOM 184 CB ASN 179 4.362 2.974 8.943 10.0 44.3 ATOM 185 CG ASN 179 5.817 2.871 9.368 1.00 44.3 ATOM 186 OD1 ASN 179 6.129 2.768 10.564 1.00 44.3 ATOM 187 ND2 ASN 179 4.078 5.458 8.823 1.00 25.8 ATOM 189 O ASN 179 4.078 5.458 8.823 1.00 25.8 ATOM 191 CA ALA 180 4.740 7.818 9.126 1.00 45.2 ATOM 193 C ALA 180 5.931 7.808 8.170 1.00 45.2 ATOM 194 O ALA 180 5.931 7.808 8.170 1.00 45.2 ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 197 CB ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 199 O ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 199 CB ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 199 CB ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 199 CB ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 CB ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 CB ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 CB ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 190 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5				-1.147 3.145 6.584 1.00 24.74
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ATOM 178 OG1 THR 178		ATOM		-0.736 3.440 11.323 1.00 19.76
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ATOM 191 CA ALA 180	35	ATOM	189 O ASN 179	
ATOM 192 CB ALA 180 5.026 8.743 10.313 1.00 36 ATOM 193 C ALA 180 5.931 7.808 8.170 1.00 45.2 40 ATOM 194 O ALA 180 6.918 7.097 8.372 1.00 36.1 ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50.0 ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM	190 N ALA 180	• • • • • • • • • • • • • • • • • • • •
ATOM 193 C ALA 180 5.931 7.808 8.170 1.00 45.2 40 ATOM 194 O ALA 180 6.918 7.097 8.372 1.00 36.1 ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50. ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM		
40 ATOM 194 O ALA 180 6.918 7.097 8.372 1.00 36.1 ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50. ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 203 O GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM		
ATOM 195 N ALA 181 5.784 8.552 7.080 1.00 44.0 ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44.0 ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50. ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM	193 C ALA 180	
ATOM 196 CA ALA 181 6.834 8.661 6.072 1.00 44. ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50. ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5	40	ATOM		
ATOM 197 CB ALA 181 8.170 9.116 6.722 1.00 50. ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM	195 N ALA 181	
ATOM 198 C ALA 181 7.069 7.427 5.196 1.00 44.0 45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM	196 CA ALA 181	
45 ATOM 199 O ALA 181 7.663 7.550 4.118 1.00 50.2 ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM	197 CB ALA 181	
ATOM 200 N GLY 182 6.567 6.268 5.622 1.00 39.0 ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39.0 ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM		
ATOM 201 CA GLY 182 6.756 5.040 4.867 1.00 39. ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5	45	ATOM		
ATOM 202 C GLY 182 8.202 4.769 4.482 1.00 39.0 ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM		
ATOM 203 O GLY 182 9.096 4.785 5.334 1.00 48.5		ATOM		
				
50 ATOM 204 N SER 183 8.438 4.564 3.189 1.00 64.5				
	50	ATOM	204 N SER 183	8.438 4.564 3.189 1.00 64.55

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	ATOM	205 CA SER 183	9.781 4.270 2.693 1.00 64.55
	ATOM	206 CB SER 183	9.690 3.402 1.430 1.00 67.68
	ATOM	207 OG SER 183	8.822 3.978 0.467 1.00 67.68
	ATOM	208 C SER 183	10.643 5.510 2.437 1.00 64.55
5	ATOM	209 O SER 183	11.839 5.407 2.158 1.00 67.68
	ATOM	210 N HIS 184	10.035 6.683 2.579 1.00 52.73
	ATOM	211 CA HIS 184	10.725 7.953 2.352 1.00 52.73
	ATOM	212 CB HIS 184	9.772 8.955 1.698 1.00 44.77
	ATOM	213 C HIS 184	11.364 8.582 3.595 1.00 52.73
10	ATOM		11.837 9.722 3.540 1.00 44.77
	ATOM	215 N TRP 185	11.420 7.842 4.699 1.00 54.14
	ATOM	216 CA TRP 185	11.977 8.389 5.940 1.00 54.14
	ATOM	217 CB TRP 185	11.813 7.395 7.104 1.00 40.24
	ATOM	218 CG TRP 185	12.605 6.123 6.991 1.00 40.24
15	ATOM	219 CD2 TRP 185	13.894 5.873 7.551 1.00 40.24
	ATOM	220 CE2 TRP 185	14.245 4.543 7.221 1.00 40.24
	ATOM	221 CE3 TRP 185	14.791 6.641 8.300 1.00 40.24
	ATOM	222 CD1 TRP 185	12.227 4.973 6.359 1.00 40.24
	ATOM	223 NE1 TRP 185	13.210 4.015 6.496 1.00 40.24
20	ATOM	224 CZ2 TRP 185	15.461 3.968 7.619 1.00 40.24
-	ATOM	225 CZ3 TRP 185	15.996 6.073 8.696 1.00 40.24
	ATOM	226 CH2 TRP 185	16.319 4.747 8.353 1.00 40.24
	ATOM	227 C TRP 185	13.432 8.870 5.819 1.00 54.14
	ATOM	228 O TRP 185	13.759 10.008 6.168 1.00 40.24
25	ATOM	229 N LYS 186	14.277 8.032 5.232 1.00 43.72
	ATOM	230 CA LYS 186	15.694 8.329 5.035 1.00 43.72
	ATOM	231 CB LYS 186	16.353 7.168 4.282 1.00 64.14
	ATOM	232 CG LYS 186	17.830 7.355 3.945 1.00 64.14
	ATOM	233 CD LYS 186	18.758 7.175 5.139 1.00 64.14
30	ATOM	234 CE LYS 186	20.195 7.060 4.652 1.00 64.14
	ATOM	235 NZ LYS 186	20.348 5.838 3.805 1.00 64.14
	ATOM	236 C LYS 186	15.900 9.634 4.263 1.00 43.72
	ATOM	237 O LYS 186	16.948 10.256 4.366 1.00 64.14
	ATOM	238 N GLN 187	14.892 10.032 3.491 1.00 58.06
35	ATOM	239 CA GLN 187	14.958 11.244 2.682 1.00 58.06
	ATOM	240 CB GLN 187	14.288 10.997 1.321 1.00 74.68
	ATOM	241 CG GLN 187	14.639 9.662 0.667 1.00 74.68
	ATOM	242 CD GLN 187	16.133 9.397 0.607 1.00 74.68
	ATOM	243 OE1 GLN 187	16.926 10.312 0.381 1.00 74.68
40	ATOM	244 NE2 GLN 187	16.528 8.156 0.855 1.00 74.68
	ATOM	245 C GLN 187	14.322 12.466 3.342 1.00 58.06
	ATOM	246 O GLN 187	14.897 13.551 3.358 1.00 74.68
	ATOM	247 N ARG 188	13.117 12.280 3.866 1.00 54.11
	ATOM	248 CA ARG 188	12.363 13.360 4.505 1.00 54.11
45	ATOM	249 CB ARG 188	10.889 13.115 4.334 1.00 53.33
	ATOM	250 C ARG 188	12.654 13.626 5.977 1.00 54.11
	ATOM	251 O ARG 188	11.879 14.298 6.659 1.00 53.33
	ATOM	252 N ARG 189	13.754 13.090 6.473 1.00 39.52
	ATOM	253 CA ARG 189	14.089 13.271 7.875 1.00 39.52
50	ATOM	254 CB ARG 189	14.594 11.959 8.482 1.00 60.85

	ATOM	255 CG ARG 189	15.969 11.555 7.991 1.00 60.85
	ATOM	256 CD ARG 189	16.442 10.298 8.693 1.00 60.85
	ATOM	257 NE ARG 189	17.833 9.963 8.385 1.00 60.85
	ATOM	258 CZ ARG 189	18.627 9.261 9.190 1.00 60.85
5	ATOM	259 NH1 ARG 189	18.178 8.805 10.356 1.00 60.85
,	ATOM	260 NH2 ARG 189	19.882 9.021 8.841 1.00 60.85
	ATOM	261 C ARG 189	15.109 14.378 8.109 1.00 39.52
	ATOM	262 O ARG 189	16.037 14.565 7.320 1.00 60.85
	ATOM	263 N LYS 190	14.934 15.100 9.212 1.00 44.13
10	ATOM	264 CA LYS 190	15.834 16.183 9.586 1.00 44.13
10	ATOM	265 CB LYS 190	15.068 17.500 9.680 1.00 45.33
	ATOM	266 C LYS 190	16.472 15.846 10.928 1.00 44.13
	ATOM	267 O LYS 190	15.827 15.272 11.805 1.00 45.33
			17.748 16.184 11.067 1.00 35.64
	ATOM		18.489 15.928 12.291 1.00 35.64
15	ATOM	269 CA PHE 191	19.993 16.008 12.025 1.00 53.94
	ATOM	270 CB PHE 191	
	ATOM	271 CG PHE 191	20.550 14.827 11.286 1.00 53.94
	ATOM	272 CD1 PHE 191	20.209 14.596 9.958 1.00 53.94
	ATOM	273 CD2 PHE 191	21.430 13.949 11.915 1.00 53.94 20.735 13.510 9.265 1.00 53.94
20	ATOM	274 CE1 PHE 191	
	ATOM	275 CE2 PHE 191	21.964 12.859 11.230 1.00 53.94 21.615 12.639 9.900 1.00 53.94
	ATOM	276 CZ PHE 191	21.615 12.639 9.900 1.00 53.94 18.135 16.928 13.384 1.00 35.64
	ATOM	277 C PHE 191	
	ATOM	278 O PHE 191	17.997 18.127 13.120 1.00 53.94
25	ATOM	279 N LEU 192	17.978 16.439 14.610 1.00 44.53
	ATOM	280 CA LEU 192	17.683 17.315 15.736 1.00 44.53
	ATOM	281 CB LEU 192	17.326 16.493 16.980 1.00 22.94
	ATOM	282 CG LEU 192	16.931 17.259 18.246 1.00 22.94
	ATOM	283 CD1 LEU 192	15.568 17.906 18.064 1.00 22.94
30	ATOM	284 CD2 LEU 192	16.909 16.308 19.427 1.00 22.94
	ATOM	285 C LEU 192	18.974 18.101 15.980 1.00 44.53
	ATOM	286 O LEU 192	20.049 17.507 16.129 1.00 22.94
	ATOM	287 N PRO 193	18.895 19.444 15.977 1.00 34.26
	ATOM	288 CD PRO 193	17.670 20.241 15.781 1.00 46.23
35	ATOM	289 CA PRO 193	20.058 20.311 16.198 1.00 34.26
	ATOM	290 CB PRO 193	19.417 21.670 16.465 1.00 46.23
	ATOM	291 CG PRO 193	18.213 21.641 15.579 1.00 46.23
	ATOM	292 C PRO 193	20.917 19.844 17.372 1.00 34.26
	ATOM	293 O PRO 193	20.413 19.614 18.471 1.00 46.23
40	ATOM	294 N ASP 194	22.217 19.716 17.125 1.00 42.67
	ATOM	295 CA ASP 194	23.174 19.254 18.128 1.00 42.67
	ATOM	296 CB ASP 194	24.583 19.226 17.536 1.00 68.50
	ATOM	297 CG ASP 194	24.731 18.185 16.450 1.00 68.50
	ATOM	298 OD1 ASP 194	25.066 17.027 16.782 1.00 68.50
45	ATOM	299 OD2 ASP 194	24.498 18.518 15.269 1.00 68.50
	ATOM	300 C ASP 194	23.187 20.003 19.457 1.00 42.67
	ATOM	301 O ASP 194	23.545 19.432 20.486 1.00 68.50
	ATOM	302 N ASP 195	22.817 21.280 19.438 1.00 47.52
	ATOM	303 CA ASP 195	22.793 22.070 20.666 1.00 47.52
50	ATOM	304 CB ASP 195	22.586 23.559 20.351 1.00 85.02

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ATOM
             305 CG ASP 195
                                21.327 23.824 19.537 1.00 85.02
     ATOM
             306 OD1 ASP 195
                                 20.291 24.188 20.138 1.00 85.02
             307 OD2 ASP 195
                                 21.377 23.683 18.294 1.00 85.02
     ATOM
             308 C ASP 195
                               21.715 21.561 21.627 1.00 47.52
     ATOM
             309 O ASP 195
                               21.762 21.826 22.831 1.00 85.02
     ATOM
             310 N ILE 196
                               20.760 20.810 21.089 1.00 44.54
     ATOM
                               19.663 20.259 21.875 1.00 44.54
             311 CA ILE 196
     ATOM
            312 CB ILE 196
                               18.379 20.137 21.023 1.00 39.66
     ATOM
                                17.223 19.627 21.874 1.00 39.66
            313 CG2 ILE 196
     ATOM
                                18.031 21.496 20.407 1.00 39.66
             314 CG1 ILE 196
10
     ATOM
                                16.816 21.475 19.503 1.00 39.66
     ATOM
             315 CD1 ILE 196
                              20.030 18.882 22.420 1.00 44.54
     ATOM
            316 C ILE 196
                               20.582 18.046 21.705 1.00 39.66
     ATOM
            317 O ILE 196
                                19.714 18.652 23.690 1.00 42.85
     ATOM
             318 N GLY 197
                                20.006 17.372 24.307 1.00 42.85
15
     ATOM
             319 CA GLY 197
             320 C GLY 197
                                21.371 17.285 24.956 1.00 42.85
     ATOM
             321 O GLY 197
                                21.815 16.198 25.318 1.00 40.22
     ATOM
                                22.029 18.425 25.137 1.00 53.07
     ATOM
             322 N GLN 198
                                23.351 18.444 25.754 1.00 53.07
     ATOM
            323 CA GLN 198
20
             324 CB GLN 198
                                24.357 19.103 24.810 1.00 44.23
     ATOM
            325 C GLN 198
                                23.344 19.153 27.110 1.00 53.07
     ATOM
            326 O GLN 198
                                24.396 19.545 27.616 1.00 44.23
     ATOM
                               22.170 19.244 27.729 1.00 35.30
             327 N SER 199
     ATOM
                                22.037 19.918 29.019 1.00 35.30
     ATOM
             328 CA SER 199
                                21.472 21.328 28.806 1.00 58.72
25
     ATOM
             329 CB SER 199
            330 OG SER 199
                                22.093 21.971 27.704 1.00 58.72
     ATOM
     ATOM
             331 C SER 199
                               21.168 19.169 30.036 1.00 35.30
     ATOM
             332 O SER 199
                               20.135 19.681 30.482 1.00 58.72
                                21.544 17.928 30.387 1.00 34.70
     ATOM
             333 N PRO 200
                                22.656 17.108 29.872 1.00 38.71
30
     ATOM
             334 CD PRO 200
             335 CA PRO 200
     ATOM
                                20.740 17.184 31.362 1.00 34.70
     ATOM
             336 CB PRO 200
                                21.311 15.769 31.266 1.00 38.71
     ATOM
             337 CG PRO 200
                                22.737 15.992 30.878 1.00 38.71
     ATOM
             338 C PRO 200
                               20.923 17.784 32.759 1.00 34.70
35
     ATOM
             339 O PRO 200
                               22.006 17.692 33.341 1.00 38.71
     ATOM
             340 N ILE 201
                               19.876 18.413 33.286 1.00 42.94
             341 CA ILE 201
                                19.961 19.041 34.604 1.00 42.94
     ATOM
     ATOM
             342 CB ILE 201
                               20.059 20.582 34.491 1.00 51.32
     ATOM
            343 CG2 ILE 201
                                21.468 20.991 34.078 1.00 51.32
             344 CG1 ILE 201
                                19.009 21.111 33.510 1.00 51.32
40
     ATOM
                                19.169 22.582 33.164 1.00 51.32
     ATOM
             345 CD1 ILE 201
     ATOM
             346 C ILE 201
                               18.871 18.676 35.610 1.00 42.94
             347 O ILE 201
                               19.049 18.875 36.814 1.00 51.32
     ATOM
             348 N VAL 202
                                17.737 18.172 35.133 1.00 50.33
     ATOM
                                 16.661 17.787 36.043 1.00 50.33
45
     ATOM
             349 CA VAL 202
                                 15.296 17.722 35.326 1.00 36.59
     ATOM
             350 CB VAL 202
     ATOM
            351 CG1 VAL 202
                                 14.202 17.311 36.304 1.00 36.59
     ATOM
             352 CG2 VAL 202
                                 14,968 19.074 34.714 1.00 36.59
             353 C VAL 202
                                17.007 16.435 36.665 1.00 50.33
     ATOM
             354 O VAL 202
                                17.335 15.481 35.955 1.00 36.59
50
     ATOM
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	ATOM	355 N SER 203	16.960 16.375 37.991 1.00 49.46
	ATOM	356 CA SER 203	17.289 15.166 38.736 1.00 49.46
	ATOM	357 CB SER 203	17.298 15.467 40.241 1.00 64.20
	ATOM	358 OG SER 203	17.673 14.330 41.003 1.00 64.20
5	ATOM	359 C SER 203	16.356 13.992 38.463 1.00 49.46
	ATOM	360 O SER 203	15.147 14.166 38.310 1.00 64.20
	ATOM	361 N MET 204	16.944 12.800 38.419 1.00 41.99
	ATOM	362 CA MET 204	16.223 11.551 38.205 1.00 41.99
	ATOM	363 CB MET 204	16.320 11.096 36.746 1.00 48.64
10	ATOM	364 CG MET 204	15.470 11.895 35.771 1.00 48.64
	ATOM	365 SD MET 204	13.702 11.783 36.114 1.00 48.64
	ATOM	366 CE MET 204	13.284 10.257 35.264 1.00 48.64
	ATOM	367 C MET 204	16.900 10.528 39.109 1.00 41.99
	ATOM	368 O MET 204	18.127 10.417 39.121 1.00 48.64
15	ATOM	369 N PRO 205	16.108 9.754 39.869 1.00 38.42
	ATOM	370 CD PRO 205	14.633 9.815 39.866 1.00 52.20
	ATOM	371 CA PRO 205	16.586 8.724 40.797 1.00 38.42
	ATOM	372 CB PRO 205	15.334 7.888 41.041 1.00 52.20
	ATOM	373 CG PRO 205	14.254 8.919 41.028 1.00 52.20
20	ATOM	374 C PRO 205	17.769 7.858 40.340 1.00 38.42
20	ATOM	375 O PRO 205	18.724 7.675 41.092 1.00 52.20
	ATOM	376 N ASP 206	17.720 7.349 39.111 1.00 49.06
	ATOM	377 CA ASP 206	18.791 6.490 38.601 1.00 49.06
	ATOM	378 CB ASP 206	18.282 5.627 37.437 1.00 74.42
25	ATOM	379 CG ASP 206	17.690 6.450 36.305 1.00 74.42
	ATOM	380 OD1 ASP 206	18.397 7.335 35.770 1.00 74.42
	ATOM	381 OD2 ASP 206	16.516 6.199 35.948 1.00 74.42
	ATOM	382 C ASP 206	20.106 7.177 38.214 1.00 49.06
	ATOM	383 O ASP 206	21.069 6.506 37.838 1.00 74.42
30	ATOM	384 N GLY 207	20.139 8.505 38.272 1.00 42.48
	ATOM	385 CA GLY 207	21.355 9.225 37.928 1.00 42.48
	ATOM	386 C GLY 207	21.330 9.965 36.601 1.00 42.48
	ATOM	387 O GLY 207	21.890 11.058 36.494 1.00 42.50
	ATOM	388 N ASP 208	20.725 9.365 35.581 1.00 46.70
35	ATOM	389 CA ASP 208	20.636 9.999 34.266 1.00 46.70
	ATOM	390 CB ASP 208	20.162 8.994 33.212 1.00 61.56
	ATOM	391 CG ASP 208	21.143 7.856 33.006 1.00 61.56
	ATOM	392 OD1 ASP 208	20.723 6.684 33.122 1.00 61.56
	ATOM	393 OD2 ASP 208	22.330 8.134 32.724 1.00 61.56
40	ATOM	394 C ASP 208	19.666 11.176 34.339 1.00 46.70
	ATOM	395 O ASP 208	18.462 10.983 34.506 1.00 61.56
	ATOM	396 N LYS 209	20,200 12,389 34,238 1.00 41.30
	ATOM	397 CA LYS 209	19,389 13.602 34.308 1.00 41.30
	ATOM	398 CB LYS 209	20.254 14.782 34.732 1.00 41.38
45	ATOM	399 C LYS 209	18.657 13.916 33.004 1.00 41.30
,,,	ATOM	400 O LYS 209	19.052 13.458 31.930 1.00 41.38
	ATOM	401 N VAL 210	17.603 14.723 33.109 1.00 43.36
	ATOM	402 CA VAL 210	16.792 15.107 31.954 1.00 43.36
	ATOM	403 CB VAL 210	15.275 15.014 32.282 1.00 30.23
50	ATOM	404 CG1 VAL 210	14.440 15.358 31.055 1.00 30.23
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14.923 13.624 32.782 1.00 30.23
            405 CG2 VAL 210
     ATOM
                               17.088 16.522 31.442 1.00 43.36
             406 C VAL 210
     ATOM
                               17.395 17.430 32.221 1.00 30.23
            407 O VAL 210
     ATOM
                               17.004 16.685 30.125 1.00 27.49
            408 N ASP 211
     ATOM
                               17.217 17.966 29.458 1.00 27.49
            409 CA ASP 211
     ATOM
                               18.073 17.765 28.198 1.00 30.75
     ATOM
            410 CB ASP 211
                               18.360 19.068 27.447 1.00 30.75
            411 CG ASP 211
     ATOM
                                19.473 19.196 26.900 1.00 30.75
            412 OD1 ASP 211
     ATOM
                                17.484 19.955 27.370 1.00 30.75
            413 OD2 ASP 211
     ATOM
                               15.819 18.445 29.073 1.00 27.49
10
     ATOM
            414 C ASP 211
                               15.197 17.892 28.166 1.00 30.75
            415 O ASP 211
     ATOM
                               15.343 19.488 29.745 1.00 31.99
     ATOM
            416 N LEU 212
                               14.013 20.042 29.492 1.00 31.99
     ATOM
            417 CA LEU 212
                                13.778 21.274 30.369 1.00 35.19
            418 CB LEU 212
     ATOM
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	ATOM	460 OE1 GLU 217	11.660 21.581 20.281 1.00 47.68
	ATOM	461 OE2 GLU 217	12.542 20.465 18.606 1.00 47.68
	ATOM	462 C GLU 217	10.505 17.044 21.179 1.00 28.84
	ATOM	463 O GLU 217	9.751 16.886 20.217 1.00 47.68
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	ATOM	465 CA PHE 218	10.259 14.725 21.883 1.00 21.49
	ATOM	466 CB PHE 218	11.020 13.746 22.781 1.00 24.12
	ATOM	467 CG PHE 218	12.489 13.652 22.464 1.00 24.12
	ATOM	468 CD1 PHE 218	13.431 13.554 23.481 1.00 24.12
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	ATOM	470 CE1 PHE 218	14.793 13.484 23.187 1.00 24.12
	ATOM	471 CE2 PHE 218	14.290 13.607 20.843 1.00 24.12
	ATOM	472 CZ PHE 218	15.221 13.511 21.867 1.00 24.12
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	ATOM	476 CA THR 219	6.949 15.231 23.685 1.00 20.07
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	ATOM	478 OG1 THR 219	7.418 17.021 25.274 1.00 28.98
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	ATOM	480 C THR 219	6.080 16.011 22.696 1.00 20.07
	ATOM	481 O THR 219	4.914 15.670 22.482 1.00 28.98
	ATOM	482 N LYS 220	6.662 17.022 22.060 1.00 25.35 5.943 17.840 21.088 1.00 25.35
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30	ATOM	484 CB LYS 220	5.414 17.015 19.916 1.00 25.35
	ATOM ATOM	485 C LYS 220 486 O LYS 220	4.376 17.343 19.339 1.00 29.07
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	ATOM	488 CA ILE 221	5.708 15.089 18.458 1.00 31.43
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	ATOM	498 CG2 ILE 222	4.221 12.545 23.145 1.00 27.10
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	ATOM	500 CD1 ILE 222	6.062 10.053 23.646 1.00 27.10
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	ATOM	503 N THR 223	2.378 12.861 20.642 1.00 33.16
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	ATOM	512 CA PRO 224 0.590 11.805 16.802 1.00 18.75
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	ATOM	518 CA ALA 225 3.040 8.916 17.300 1.00 12.19
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	ATOM	520 C ALA 225 2.187 7.881 18.030 1.00 12.19
	ATOM	521 O ALA 225 1.998 6.764 17.545 1.00 20.39
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	ATOM	532 CB THR 227 -2.706 9.360 17.207 1.00 22.37
	ATOM	533 OG1 THR 227 -2.890 10.301 18.273 1.00 22.37
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	ATOM	536 O THR 227 -3.091 6.217 16.402 1.00 22.37
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	ATOM	545 NH2 ARG 228 3.864 10.716 13.374 1.00 33.87
	ATOM	546 C ARG 228 -0.813 4.531 15.516 1.00 14.49
	ATOM	547 O ARG 228 -1.309 3.632 14.839 1.00 33.87
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	ATOM	551 CG1 VAL 229 0.339 1.612 19.350 1.00 13.78
	ATOM	552 CG2 VAL 229 1.915 3.312 18.430 1.00 13.78
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50	ATOM	554 O VAL 229 -2.185 1.465 17.323 1.00 13.78

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	ATOM	757 CA MET 256	
_	ATOM	758 CB MET 256	6.515 2.218 25.423 1.00 19.23
5	ATOM	759 CG MET 256	7.988 2.607 25.477 1.00 19.23
	ATOM	760 SD MET 256	8.344 4.132 24.571 1.00 19.23 10.127 4.254 24.782 1.00 19.23
	ATOM	761 CE MET 256	
	ATOM	762 C MET 256	6.734 0.978 23.246 1.00 13.77
• •	ATOM	763 O MET 256	7.672 1.284 22.516 1.00 19.23 6.316 -0.275 23.400 1.00 12.57
10	ATOM	764 N GLU 257	6.971 -1.397 22.730 1.00 12.57
	ATOM	765 CA GLU 257	6.342 -2.716 23.182 1.00 31.54
	ATOM	766 CB GLU 257	
	ATOM	767 CG GLU 257	6.497 -2.982 24.677 1.00 31.54
	ATOM	768 CD GLU 257	5.720 -4.196 25.167 1.00 31.54
15	ATOM	769 OE1 GLU 257	5.220 -4.983 24.334 1.00 31.54
	ATOM	770 OE2 GLU 257	5.607 -4.361 26.400 1.00 31.54 6.889 -1.254 21.211 1.00 12.57
	ATOM	771 C GLU 257	
	ATOM	772 O GLU 257	7.881 -1.452 20.505 1.00 31.54
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	ATOM	775 CB ILE 258	3.813 -0.129 17.493 1.00 15.57
	ATOM	776 CG2 ILE 258 777 CG1 ILE 258	3.288 -1.886 19.211 1.00 15.57
	ATOM		1.798 -1.872 18.922 1.00 15.57
25	ATOM ATOM	778 CD1 ILE 258 779 C ILE 258	6.289 0.535 18.811 1.00 17.89
23	ATOM	780 O ILE 258	7.000 0.468 17.805 1.00 15.57
	ATOM	781 N MET 259	6.196 1.636 19.556 1.00 11.23
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	ATOM	783 CB MET 259	6.568 3.995 20.175 1.00 22.19
30	ATOM	784 CG MET 259	5.112 4.439 20.117 1.00 22.19
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	ATOM	786 CE MET 259	5.038 5.606 22.621 1.00 22.19
	ATOM	787 C MET 259	8.415 2.637 19.131 1.00 11.23
	ATOM	788 O MET 259	9.060 3.008 18.145 1.00 22.19
35	ATOM	789 N SER 260	8.974 1.994 20.153 1.00 8.59
	ATOM	790 CA SER 260	10.408 1.706 20.195 1.00 8.59
	ATOM	791 CB SER 260	10.763 0.939 21.472 1.00 23.39
	ATOM	792 OG SER 260	10.430 1.685 22.623 1.00 23.39
	ATOM	793 C SER 260	10.793 0.864 18.977 1.00 8.59
40	ATOM	794 O SER 260	11.824 1.100 18.350 1.00 23.39
-	ATOM	795 N LEU 261	9.952 -0.111 18.644 1.00 13.26
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	ATOM	797 CB LEU 261	9.076 -2.035 17.401 1.00 14.32
	ATOM	798 CG LEU 261	9.019 -2.894 16.134 1.00 14.32
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     ATOM 904 CA THR 275
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	ATOM	906 OG1 THR 275	15.622 7.983 11.228 1.00 37.64
	ATOM	907 CG2 THR 275	13.570 9.215 11.222 1.00 37.64
	ATOM	908 C THR 275	13.120 8.135 14.032 1.00 27.89
5	ATOM	909 O THR 275	12.493 7.081 14.019 1.00 37.64
	ATOM	910 N LEU 276	12.700 9.226 14.667 1.00 28.07
	ATOM	911 CA LEU 276	11.418 9.275 15.358 1.00 28.07
	ATOM	912 CB LEU 276	11.497 10.214 16.572 1.00 24.81
	ATOM	913 CG LEU 276	12.639 10.005 17.577 1.00 24.81
10	ATOM	914 CD1 LEU 276	12.450 10.929 18.769 1.00 24.81
	ATOM	915 CD2 LEU 276	12.692 8.558 18.038 1.00 24.81
	ATOM	916 C LEU 276	10.339 9.761 14.395 1.00 28.07
	ATOM	917 O LEU 276	10.533 10.760 13.691 1.00 24.81
	ATOM	918 N SER 277	9.232 9.027 14.331 1.00 29.24
15	ATOM	919 CA SER 277	8.106 9.357 13.458 1.00 29.24
	ATOM	920 CB SER 277	7.369 10.594 13.985 1.00 30.56
	ATOM	921 OG SER 277	6.845 10.358 15.283 1.00 30.56
	ATOM	922 C SER 277	8.533 9.569 12.005 1.00 29.24
	ATOM	923 O SER 277	7.902 10.326 11.263 1.00 30.56
20	ATOM	924 N GLY 278	9.619 8.908 11.618 1.00 34.41
	ATOM	925 CA GLY 278	10.135 9.024 10.263 1.00 34.41
	ATOM	926 C GLY 278	10.472 10.442 9.830 1.00 34.41
	ATOM	927 O GLY 278	10.516 10.725 8.631 1.00 44.04
	ATOM	928 N GLU 279	10.733 11.326 10.791 1.00 37.82
25	ATOM	929 CA GLU 279	11.056 12.717 10.479 1.00 37.82
	ATOM	930 CB GLU 279	9.808 13.600 10.612 1.00 70.24
	ATOM	931 CG GLU 279	9.202 13.631 12.014 1.00 70.24
	ATOM	932 CD GLU 279	8.028 14.593 12.141 1.00 70.24
	ATOM	933 OE1 GLU 279	8.028 15.406 13.093 1.00 70.24
30	ATOM	934 OE2 GLU 279	7.103 14.535 11.301 1.00 70.24
	ATOM	935 C GLU 279	12.192 13.321 11.300 1.00 37.82
	ATOM	936 O GLU 279	12.857 14.248 10.841 1.00 70.24
	ATOM	937 N MET 280	12.424 12.811 12.505 1.00 33.77
	ATOM	938 CA MET 280	13.482 13.360 13.344 1.00 33.77
35	ATOM	939 CB MET 280	12.903 13.848 14.674 1.00 33.89
	ATOM	940 CG MET 280	13.898 14.595 15.545 1.00 33.89
	ATOM	941 SD MET 280	13.350 14.740 17.256 1.00 33.89
	ATOM	942 CE MET 280	12.100 16.017 17.121 1.00 33.89
	ATOM	943 C MET 280	14.620 12.383 13.613 1.00 33.77
40	ATOM	944 O MET 280	14.432 11.366 14.282 1.00 33.89
	ATOM	945 N ALA 281	15.797 12.690 13.080 1.00 30.24
	ATOM	946 CA ALA 281	16.972 11.852 13.287 1.00 30.24
	ATOM	947 CB ALA 281	17.937 11.998 12.120 1.00 25.10
	ATOM	948 C ALA 281	17.631 12.309 14.587 1.00 30.24
45	ATOM	949 O ALA 281	18.008 13.477 14.718 1.00 25.10
	ATOM	950 N VAL 282	17.743 11.401 15.551 1.00 32.12
	ATOM	951 CA VAL 282	18.339 11.726 16.844 1.00 32.12
	ATOM	952 CB VAL 282	17.303 11.606 17.991 1.00 37.75
50	ATOM	953 CG1 VAL 282	16.184 12.615 17.799 1.00 37.75
50	ATOM	954 CG2 VAL 282	16.739 10.193 18.055 1.00 37.75

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                               19.543 10.852 17.181 1.00 32.12
            956 O VAL 282
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     ATOM
            957 N LYS 283
                               20.491 11.428 17.913 1.00 26.82
     ATOM
            958 CA LYS 283
                               21.700 10.722 18.328 1.00 26.82
     ATOM
            959 CB LYS 283
                               22.894 11.679 18.342 1.00 57.25
     ATOM
            960 CG LYS 283
                               23.258 12.245 16.979 1.00 57.25
     ATOM
                               24.282 13.361 17.105 1.00 57.25
            961 CD LYS 283
     ATOM
            962 CE LYS 283
                               24.752 13.836 15.741 1.00 57.25
     ATOM
            963 NZ LYS 283
                               25.518 12.772 15.033 1.00 57.25
     ATOM
                              21.509 10.120 19.717 1.00 26.82
            964 C LYS 283
10
     ATOM
                               20,648 10,566 20,477 1.00 57.25
            965 O LYS 283
     ATOM
            966 N ARG 284
                               22.351 9.146 20.058 1.00 26.41
     ATOM
            967 CA ARG 284
                                22.297 8.457 21.351 1.00 26.41
     ATOM
     ATOM
            968 CB ARG 284
                                23.527 7.566 21.528 1.00 41.02
15
     ATOM
            969 CG ARG 284
                                23.715 6.539 20.440 1.00 41.02
            970 CD ARG 284
     ATOM
                                25.016 5.794 20.616 1.00 41.02
            971 NE ARG 284
                                25.145 4.730 19.630 1.00 41.02
     ATOM
                                24.759 3.475 19.831 1.00 41.02
     ATOM
            972 CZ ARG 284
            973 NH1 ARG 284
                                24.221 3.117 20.990 1.00 41.02
     ATOM
                                24.886 2.584 18.859 1.00 41.02
20
     ATOM
            974 NH2 ARG 284
            975 C ARG 284
                               22.200 9.399 22.543 1.00 26.41
     ATOM
            976 O ARG 284
                               21.296 9.278 23.370 1.00 41.02
     ATOM
            977 N GLU 285
                               23.152 10.321 22.634 1.00 33.23
     ATOM
            978 CA GLU 285
     ATOM
                                23.201 11.292 23.721 1.00 33.23
                                24.366 12.258 23.492 1.00 69.82
            979 CB GLU 285
25
     ATOM
            980 CG GLU 285
                                24.485 13.359 24.533 1.00 69.82
     ATOM
     ATOM
            981 CD GLU 285
                                25.079 14.636 23.964 1.00 69.82
     ATOM
            982 OE1 GLU 285
                                26.309 14.826 24.070 1.00 69.82
     ATOM
            983 OE2 GLU 285
                                24.309 15.453 23.409 1.00 69.82
30
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            984 C GLU 285
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            985 O GLU 285
     ATOM
                               21.336 12.239 24.907 1.00 69.82
     ATOM
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                               21.414 12.551 22.677 1.00 28.07
     ATOM
            987 CA GLN 286
                                20.194 13.346 22.614 1.00 28.07
     ATOM
            988 CB GLN 286
                                19.948 13.824 21.181 1.00 41.05
                                21.051 14.726 20.639 1.00 41.05
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     ATOM
            989 CG GLN 286
     ATOM
            990 CD GLN 286
                                20.808 15.154 19.202 1.00 41.05
            991 OEI GLN 286
                                20.783 14.322 18.293 1.00 41.05
     ATOM
     ATOM 992 NE2 GLN 286
                                20.635 16.452 18.990 1.00 41.05
            993 C GLN 286
                               18.955 12.642 23.162 1.00 28.07
     ATOM
            994 O GLN 286
                               18.281 13.174 24.048 1.00 41.05
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     ATOM
     ATOM
            995 N LEU 287
                               18.663 11.447 22.658 1.00 30.11
                               17.492 10.705 23.116 1.00 30.11
            996 CA LEU 287
     ATOM
            997 CB LEU 287
                                17.232 9.489 22.219 1.00 21.70
     ATOM
                                15.859 8.821 22.357 1.00 21.70
     ATOM
            998 CG LEU 287
45
     ATOM
            999 CD1 LEU 287
                                14.748 9.818 22.061 1.00 21.70
     ATOM 1000 CD2 LEU 287
                                15.763 7.628 21.421 1.00 21.70
     ATOM 1001 C LEU 287
                               17.641 10.277 24.577 1.00 30.11
     ATOM 1002 O LEU 287
                               16.655 10.212 25.320 1.00 21.70
     ATOM 1003 N LYS 288
                               18.878 10.015 24.992 1.00 20.72
     ATOM 1004 CA LYS 288
                                19.156 9.611 26.365 1.00 20.72
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	ATOM	1005 CB LYS 288	20.626 9.213 26.514 1.00 43.14
	ATOM	1006 CG LYS 288	20.991 8.721 27.903 1.00 43.14
	ATOM	1007 CD LYS 288	22.374 8.102 27.931 1.00 43.14
	ATOM	1008 CE LYS 288	22.615 7.379 29.250 1.00 43.14
5	ATOM	1009 NZ LYS 288	23.866 6.568 29.224 1.00 43.14
_	ATOM	1010 C LYS 288	18.819 10.742 27.331 1.00 20.72
	ATOM	1011 O LYS 288	18.027 10.566 28.261 1.00 43.14
	ATOM	1012 N ASN 289	19.380 11.917 27.067 1.00 33.64
	ATOM	1013 CA ASN 289	19.156 13.090 27.906 1.00 33.64
10	ATOM	1014 CB ASN 289	20.190 14.173 27.590 1.00 35.61
10	ATOM	1014 CB ASN 289	21.607 13.730 27.898 1.00 35.61
	ATOM	1016 OD1 ASN 289	21.835 12.920 28.797 1.00 35.61
	ATOM	1010 OD1 ASN 289	22.566 14.253 27.149 1.00 35.61
		1017 ND2 ASN 289	17.747 13.654 27.757 1.00 33.64
٠	ATOM		17.276 14.399 28.616 1.00 35.61
15	ATOM		17.276 14.399 28.616 1.06 33.61
	ATOM		15.722 13.767 26.435 1.00 22.05
	ATOM	1021 CA GLY 290	13.722 13.767 26.433 1.00 22.03
	ATOM	1022 C GLY 290	13.550 13.710 27.420 1.00 29.95
••	ATOM	1023 O GLY 290	13.550 13.710 27.420 1.00 29.93
20	ATOM	1024 N GLY 291	
	ATOM	1025 CA GLY 291	14.142 11.732 29.211 1.00 24.91
	ATOM	1026 C GLY 291	14.093 10.217 29.248 1.00 24.91
	ATOM	1027 O GLY 291	13.536 9.640 30.179 1.00 29.39
	ATOM	1028 N LEU 292	14.676 9.567 28.246 1.00 30.21
25	ATOM	1029 CA LEU 292	14.675 8.110 28.189 1.00 30.21
	ATOM	1030 CB LEU 292	14.732 7.626 26.734 1.00 21.45
	ATOM	1031 CG LEU 292	13.439 7.795 25.928 1.00 21.45
	ATOM	1032 CD1 LEU 292	13.612 7.225 24.542 1.00 21.45
	ATOM	1033 CD2 LEU 292	12.296 7.087 26.630 1.00 21.45
30	ATOM	1034 C LEU 292	15.785 7.461 29.013 1.00 30.21
	ATOM	1035 O LEU 292	15.645 6.324 29.473 1.00 21.45
	ATOM	1036 N GLY 293	16.885 8.180 29.205 1.00 16.29
	ATOM	1037 CA GLY 293	17.992 7.638 29.970 1.00 16.29
	ATOM	1038 C GLY 293	18.534 6.374 29.332 1.00 16.29
35	ATOM	1039 O GLY 293	18.763 6.334 28.122 1.00 25.88
	ATOM	1040 N VAL 294	18.689 5.322 30.130 1.00 33.05
	ATOM	1041 CA VAL 294	19.211 4.050 29.635 1.00 33.05
	ATOM	1042 CB VAL 294	19.530 3.069 30.788 1.00 30.11
	ATOM	1043 CG1 VAL 294	20.718 3.577 31.582 1.00 30.11
40	ATOM	1044 CG2 VAL 294	18.315 2.887 31.697 1.00 30.11
	ATOM	1045 C VAL 294	18.302 3.361 28.617 1.00 33.05
	ATOM	1046 O VAL 294	18.768 2.545 27.817 1.00 30.11
	ATOM	1047 N VAL 295	17.014 3.699 28.635 1.00 18.14
	ATOM	1048 CA VAL 295	16.056 3.118 27.698 1.00 18.14
45	ATOM	1049 CB VAL 295	14.638 3.698 27.902 1.00 28.34
	ATOM	1050 CG1 VAL 295	13.668 3.099 26.893 1.00 28.34
	ATOM	1051 CG2 VAL 295	14.159 3.431 29.317 1.00 28.34
	ATOM	1052 C VAL 295	16.521 3.415 26.275 1.00 18.14
	ATOM	1052 O VAL 295	16.395 2.577 25.383 1.00 28.34
50	ATOM	1054 N SER 296	17.091 4.601 26.085 1.00 20.84
50	1110141	100 (1. 0221 270	

	ATOM	1055 CA SER 296	17.596 5.028 24.785 1.00 20.84
			18.160 6.446 24.884 1.00 25.61
	ATOM ATOM	1056 CB SER 296 1057 OG SER 296	18.615 6.911 23.627 1.00 25.61
		1057 OG SER 290 1058 C SER 296	18.687 4.074 24.307 1.00 20.84
_	ATOM	1056 C SER 296	18.723 3.691 23.133 1.00 25.61
5	ATOM		19.571 3.691 25.224 1.00 28.08
	ATOM		20.660 2.777 24.904 1.00 28.08
	ATOM		
	ATOM	1062 CB ASP 297	
	ATOM	1063 CG ASP 297	22.207 3.835 26.629 1.00 51.15 22.508 4.725 25.804 1.00 51.15
10	ATOM	1064 OD1 ASP 297	
	ATOM	1065 OD2 ASP 297	22.425 3.948 27.855 1.00 51.15
	ATOM	1066 C ASP 297	20.079 1.450 24.434 1.00 28.08
	ATOM	1067 O ASP 297	20.549 0.869 23.456 1.00 51.15
	ATOM	1068 N ALA 298	19.024 1.006 25.111 1.00 26.12
15	ATOM	1069 CA ALA 298	18.357 -0.245 24.778 1.00 26.12
	ATOM	1070 CB ALA 298	17.253 -0.530 25.787 1.00 18.80
	ATOM	1071 C ALA 298	17.790 -0.223 23.356 1.00 26.12
	ATOM	1072 O ALA 298	18.014 -1.154 22.575 1.00 18.80
	ATOM	1073 N ILE 299	17.078 0.848 23.013 1.00 17.42
20	ATOM	1074 CA ILE 299	16.483 0.979 21.686 1.00 17.42
	ATOM	1075 CB ILE 299	15.559 2.211 21.597 1.00 16.69
	ATOM	1076 CG2 ILE 299	14.845 2.238 20.253 1.00 16.69
	ATOM	1077 CG1 ILE 299	14.515 2.149 22.712 1.00 16.69
	ATOM	1078 CD1 ILE 299	13.713 3.406 22.872 1.00 16.69
25	ATOM	1079 C ILE 299	17.563 1.042 20.609 1.00 17.42
	ATOM	1080 O ILE 299	17.416 0.443 19.542 1.00 16.69
	ATOM	1081 N PHE 300	18.652 1.752 20.889 1.00 14.46
	ATOM	1082 CA PHE 300	19.751 1.851 19.935 1.00 14.46
	ATOM	1083 CB PHE 300	20.804 2.854 20.409 1.00 24.01
30	ATOM	1084 CG PHE 300	20.656 4.221 19.801 1.00 24.01
	ATOM	1085 CD1 PHE 300	19.904 5.204 20.435 1.00 24.01
	ATOM	1086 CD2 PHE 300	21.271 4.526 18.591 1.00 24.01
	ATOM	1087 CE1 PHE 300	19.766 6.472 19.873 1.00 24.01
	ATOM	1088 CE2 PHE 300	21.140 5.791 18.020 1.00 24.01
35	ATOM	1089 CZ PHE 300	20.385 6.765 18.663 1.00 24.01
	ATOM	1090 C PHE 300	20.383 0.480 19.726 1.00 14.46
	ATOM	1091 O PHE 300	20.696 0.102 18.596 1.00 24.01
	ATOM	1092 N GLU 301	20.547 -0.270 20.813 1.00 21.61
	ATOM	1093 CA GLU 301	21.123 -1.609 20.744 1.00 21.61
40	ATOM	1094 CB GLU 301	21.289 -2.192 22.143 1.00 23.89
	ATOM	1095 C GLU 301	20.211 -2.498 19.904 1.00 21.61
	ATOM	1096 O GLU 301	20.681 -3.251 19.043 1.00 23.89
	ATOM	1097 N LEU 302	18.906 -2.390 20.140 1.00 14.43
	ATOM	1098 CA LEU 302	17.922 -3.168 19.399 1.00 14.43
45	ATOM	1099 CB LEU 302	16.512 -2.872 19.912 1.00 23.43
	ATOM	1100 CG LEU 302	15.350 -3.669 19.312 1.00 23.43
	ATOM	1101 CD1 LEU 302	
	ATOM	1102 CD2 LEU 302	
	ATOM	1103 C LEU 302	18.027 -2.812 17.917 1.00 14.43
50	ATOM	1104 O LEU 302	18.089 -3.697 17.066 1.00 23.43

	ATOM	1105 N GLY 303	18.098 -1.515 17.625 1.00 15.17
	ATOM	1106 CA GLY 303	18.208 -1.056 16.251 1.00 15.17
	ATOM	1107 C GLY 303	19.411 -1.640 15.530 1.00 15.17
	ATOM	1108 O GLY 303	19.290 -2.137 14.406 1.00 27.67
5	ATOM	1109 N LYS 304	20.570 -1.594 16.182 1.00 19.04
	ATOM	1110 CA LYS 304	21.802 -2.127 15.605 1.00 19.04
	ATOM	1111 CB LYS 304	22.979 -1.975 16.577 1.00 56.94
	ATOM	1112 CG LYS 304	23.496 -0.556 16.741 1.00 56.94
	ATOM	1112 CO LYS 304	24.811 -0.524 17.516 1.00 56.94
10	ATOM	1114 CE LYS 304	24.634 -0.965 18.968 1.00 56.94
10		1114 CE LTS 304 1115 NZ LYS 304	
	ATOM		
	ATOM	1116 C LYS 304	21.653 -3.596 15.229 1.00 19.04
	ATOM	1117 O LYS 304	21.974 -3.993 14.107 1.00 56.94
	ATOM	1118 N SER 305	21.146 -4.394 16.164 1.00 24.46
15	ATOM	1119 CA SER 305	20.965 -5.822 15.932 1.00 24.46
	ATOM	1120 CB SER 305	20.610 -6.533 17.240 1.00 37.46
	ATOM	1121 OG SER 305	19.444 -5.984 17.827 1.00 37.46
	ATOM	1122 C SER 305	19.926 -6.128 14.853 1.00 24.46
	ATOM	1123 O SER 305	20.146 -6.996 14.006 1.00 37.46
20	ATOM	1124 N LEU 306	18.819 -5.390 14.858 1.00 25.47
	ATOM	1125 CA LEU 306	17.753 -5.592 13.881 1.00 25.47
	ATOM	1126 CB LEU 306	16.525 -4.746 14.224 1.00 15.99
	ATOM	1127 CG LEU 306	15.700 -5.190 15.432 1.00 15.99
	ATOM	1128 CD1 LEU 306	14.504 -4.271 15.600 1.00 15.99
25	ATOM	1129 CD2 LEU 306	15.244 -6.624 15.247 1.00 15.99
	ATOM	1130 C LEU 306	18.174 -5.330 12.439 1.00 25.47
	ATOM	1131 O LEU 306	17.596 -5.902 11.513 1.00 15.99
	ATOM	1132 N SER 307	19.182 -4.482 12.247 1.00 24.28
	ATOM	1133 CA SER 307	19.670 -4.160 10.907 1.00 24.28
30	ATOM	1134 CB SER 307	20.910 -3.263 10.989 1.00 40.92
	ATOM	1135 OG SER 307	20.617 -2.028 11.622 1.00 40.92
	ATOM	1136 C SER 307	19.995 -5.422 10.107 1.00 24.28
	ATOM	1137 O SER 307	19.625 -5.535 8.936 1.00 40.92
	ATOM	1138 N ALA 308	20.644 -6.383 10.761 1.00 30.97
35	ATOM	1139 CA ALA 308	21.027 -7.640 10.124 1.00 30.97
,,,	ATOM	1140 CB ALA 308	22.004 -8.399 11.013 1.00 37.84
	ATOM	1141 C ALA 308	19.830 -8.528 9.779 1.00 30.97
	ATOM	1142 O ALA 308	19.897 -9.336 8.853 1.00 37.84
	ATOM	1142 O ALK 300 1143 N PHE 309	18.737 -8.372 10.520 1.00 22.78
40	ATOM	1144 CA PHE 309	17.533 -9.166 10.292 1.00 22.78
70	ATOM	1145 CB PHE 309	16.571 -9.037 11.477 1.00 30.14
	ATOM	1146 CG PHE 309	17.032 -9.751 12.716 1.00 30.14
	ATOM	1147 CD1 PHE 309	16.299 -10.809 13.236 1.00 30.14
			18.204 -9.372 13.359 1.00 30.14
15	ATOM	1148 CD2 PHE 309	
45	ATOM	1149 CE1 PHE 309	16.725 -11.481 14.378 1.00 30.14 18.640 -10.038 14.503 1.00 30.14
	ATOM	1150 CE2 PHE 309	
	ATOM	1151 CZ PHE 309	17.896 -11.094 15.013 1.00 30.14
	ATOM	1152 C PHE 309	16.818 -8.813 8.990 1.00 22.78
50	ATOM	1153 O PHE 309	16.068 -9.631 8.451 1.00 30.14
50	ATOM	1154 N ASN 310	17.051 -7.598 8.496 1.00 35.30

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16.441 -7.109 7.255 1.00 35.30
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                                17.109 -7.760 6.037 1.00 28.28
    ATOM 1156 CB ASN 310
    ATOM 1157 C ASN 310
                               14.929 -7.339 7.229 1.00 35.30
                               14.395 -7.970 6.312 1.00 28.28
     ATOM 1158 O ASN 310
                               14.249 -6.831 8.251 1.00 27.52
    ATOM 1159 N LEU 311
                                12.803 -6.979 8.369 1.00 27.52
    ATOM 1160 CA LEU 311
    ATOM 1161 CB LEU 311
                                12.351 -6.630 9.788 1.00 22.62
                                12.950 -7.396 10.968 1.00 22.62
    ATOM 1162 CG LEU 311
                                12.360 -6.864 12.268 1.00 22.62
    ATOM 1163 CD1 LEU 311
    ATOM 1164 CD2 LEU 311
                                12.672 -8.881 10.821 1.00 22.62
10
                               12.060 -6.085 7.382 1.00 27.52
    ATOM 1165 C LEU 311
                               12.519 -4.986 7.067 1.00 22.62
    ATOM 1166 O LEU 311
                               10.918 -6.563 6.892 1.00 16.74
    ATOM 1167 N ASP 312
                               10.095 -5.789 5.968 1.00 16.74
    ATOM 1168 CA ASP 312
    ATOM 1169 CB ASP 312
                                9.803 -6.578 4.673 1.00 16.35
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                                8.924 -7.814 4.888 1.00 16.35
    ATOM 1170 CG ASP 312
                                8.591 -8.168 6.037 1.00 16.35
    ATOM 1171 OD1 ASP 312
    ATOM 1172 OD2 ASP 312
                                 8.559 -8.446 3.876 1.00 16.35
    ATOM 1173 C ASP 312
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                               8.535 -5.798 7.797 1.00 16.35
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    ATOM 1174 O ASP 312
                               8.007 -4.520 6.019 1.00 5.43
     ATOM 1175 N ASP 313
                                6.758 -4.016 6.592 1.00 5.43
    ATOM 1176 CA ASP 313
     ATOM 1177 CB ASP 313
                                5.974 -3.201 5.559 1.00 31.80
                                6.670 -1.906 5.183 1.00 31.80
     ATOM 1178 CG ASP 313
                                 7.392 -1.340 6.033 1.00 31.80
    ATOM 1179 OD1 ASP 313
25
    ATOM 1180 OD2 ASP 313
                                 6.493 -1.452 4.032 1.00 31.80
                               5.849 -5.081 7.189 1.00 5.43
    ATOM 1181 C ASP 313
                               5.216 -4.849 8.221 1.00 31.80
    ATOM 1182 O ASP 313
                               5.777 -6.238 6.543 1.00 12.98
    ATOM 1183 N THR 314
                                4.934 -7.327 7.022 1.00 12.98
    ATOM 1184 CA THR 314
30
                                4.825 -8.441 5.968 1.00 18.90
     ATOM 1185 CB THR 314
    ATOM 1186 OG1 THR 314
                                 4.249 -7.904 4.769 1.00 18.90
                                 3.960 -9.578 6.477 1.00 18.90
    ATOM 1187 CG2 THR 314
                               5.426 -7.910 8.349 1.00 12.98
     ATOM 1188 C THR 314
35
    ATOM 1189 O THR 314
                               4.636 -8.124 9.268 1.00 18.90
                                6.731 -8.135 8.457 1.00 9.13
    ATOM 1190 N GLU 315
                                7.316 -8.685 9.675 1.00 9.13
    ATOM 1191 CA GLU 315
                                8.771 -9.078 9.427 1.00 11.49
    ATOM 1192 CB GLU 315
    ATOM 1193 CG GLU 315
                                8.870 -10.323 8.562 1.00 11.49
40
    ATOM 1194 CD GLU 315
                                10.233 -10.544 7.945 1.00 11.49
    ATOM 1195 OE1 GLU 315
                                10.964 -9.561 7.705 1.00 11.49
    ATOM 1196 OE2 GLU 315
                                10.558 -11.715 7.669 1.00 11.49
    ATOM 1197 C GLU 315
                                7.180 -7.720 10.847 1.00 9.13
    ATOM 1198 O GLU 315
                                6.863 -8.131 11.967 1.00 11.49
                                7.376 -6.433 10.575 1.00 9.46
    ATOM 1199 N VAL 316
45
    ATOM 1200 CA VAL 316
                                7.240 -5.406 11.602 1.00 9.46
                                7.655 -4.015 11.063 1.00 7.95
    ATOM 1201 CB VAL 316
    ATOM 1202 CG1 VAL 316
                                 7.434 -2.941 12.124 1.00 7.95
    ATOM 1203 CG2 VAL 316
                                 9.112 -4.037 10.625 1.00 7.95
     ATOM 1204 C VAL 316
                               5.777 -5.365 12.051 1.00 9.46
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5.484 -5.300 13.247 1.00 7.95
    ATOM 1205 O VAL 316
    ATOM 1206 N ALA 317
                               4.866 -5.438 11.083 1.00 5.52
                                3.434 -5.417 11.355 1.00 5.52
    ATOM 1207 CA ALA 317
    ATOM 1208 CB ALA 317
                                2.656 -5.415 10.054 1.00 10.98
    ATOM 1209 C ALA 317
                               3.002 -6.595 12.225 1.00 5.52
                               2.317 -6.412 13.230 1.00 10.98
    ATOM 1210 O ALA 317
    ATOM 1211 N LEU 318
                               3.411 -7.799 11.838 1.00 8.62
    ATOM 1212 CA LEU 318
                                3.067 -9.003 12.584 1.00 8.62
    ATOM 1213 CB LEU 318
                                3.523 -10.249 11.825 1.00 10.49
    ATOM 1214 CG LEU 318
                                2.770 -10.494 10.514 1.00 10.49
10
                                3.376 -11.664 9.769 1.00 10.49
    ATOM 1215 CD1 LEU 318
                                 1.297 -10.741 10.799 1.00 10.49
    ATOM 1216 CD2 LEU 318
                               3.674 -8.971 13.978 1.00 8.62
    ATOM 1217 C LEU 318
                               3.047 -9.407 14.945 1.00 10.49
    ATOM 1218 O LEU 318
    ATOM 1219 N LEU 319
                               4.885 -8.435 14.082 1.00 9.43
15
    ATOM 1220 CA LEU 319
                                5.560 -8.325 15.366 1.00 9.43
    ATOM 1221 CB LEU 319
                                6.975 -7.773 15.173 1.00 24.05
                                7.901 -7.680 16.389 1.00 24.05
    ATOM 1222 CG LEU 319
                                 7.889 -8.977 17.182 1.00 24.05
    ATOM 1223 CD1 LEU 319
20
    ATOM 1224 CD2 LEU 319
                                 9.310 -7.356 15.922 1.00 24.05
    ATOM 1225 C LEU 319
                               4.731 -7.404 16.259 1.00 9.43
                               4.456 -7.731 17.416 1.00 24.05
    ATOM 1226 O LEU 319
     ATOM 1227 N GLN 320
                                4.287 -6.282 15.699 1.00 8.67
    ATOM 1228 CA GLN 320
                                3.467 -5.325 16.437 1.00 8.67
    ATOM 1229 CB GLN 320
                                3.151 -4.102 15.573 1.00 10.94
25
                                4.361 -3.256 15.218 1.00 10.94
    ATOM 1230 CG GLN 320
    ATOM 1231 CD GLN 320
                                4.025 -2.045 14.359 1.00 10.94
                                 4.889 -1.217 14.082 1.00 10.94
     ATOM 1232 OE1 GLN 320
    ATOM 1233 NE2 GLN 320
                                 2.773 -1.940 13.924 1.00 10.94
    ATOM 1234 C GLN 320
                               2.169 -5.984 16.895 1.00 8.67
30
    ATOM 1235 O GLN 320
                                1.708 -5.751 18.013 1.00 10.94
    ATOM 1236 N ALA 321
                                1.586 -6.806 16.028 1.00 9.21
                                0.349 -7.513 16.342 1.00 9.21
     ATOM 1237 CA ALA 321
    ATOM 1238 CB ALA 321
                                -0.136 -8.283 15.129 1.00 12.83
    ATOM 1239 C ALA 321
                               0.558 -8.460 17.523 1.00 9.21
35
     ATOM 1240 O ALA 321
                               -0.315 -8.591 18.382 1.00 12.83
                                1.718 -9.111 17.566 1.00 9.10
     ATOM 1241 N VAL 322
                                2.043 -10.030 18.651 1.00 9.10
    ATOM 1242 CA VAL 322
    ATOM 1243 CB VAL 322
                                3.340 -10.827 18.352 1.00 15.92
                                 3.783 -11.614 19.575 1.00 15.92
    ATOM 1244 CG1 VAL 322
                                 3.106 -11.780 17.194 1.00 15.92
     ATOM 1245 CG2 VAL 322
     ATOM 1246 C VAL 322
                               2.192 -9.256 19.960 1.00 9.10
    ATOM 1247 O VAL 322
                                1.707 -9.691 21.003 1.00 15.92
     ATOM 1248 N LEU 323
                               2.856 -8.106 19.893 1.00 11.07
                                3.062 -7.257 21.064 1.00 11.07
    ATOM 1249 CA LEU 323
45
     ATOM 1250 CB LEU 323
                                3.959 -6.070 20.705 1.00 16.31
                                5.377 -6.393 20.229 1.00 16.31
     ATOM 1251 CG LEU 323
     ATOM 1252 CD1 LEU 323
                                 6.039 -5.149 19.669 1.00 16.31
     ATOM 1253 CD2 LEU 323
                                6.187 -6.966 21.375 1.00 16.31
                               1.729 -6.742 21.595 1.00 11.07
     ATOM 1254 C LEU 323
50
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110 //120/00			
	ATOM	1255 O LEU 323	1.523 -6.650 22.803 1.00 16.31
	ATOM	1256 N LEU 324	0.827 -6.413 20.677 1.00 13.48
	ATOM	1257 CA LEU 324	-0.494 -5.900 21.015 1.00 13.48
	ATOM	1258 CB LEU 324	-1.185 -5.383 19.752 1.00 15.92
5	ATOM	1259 CG LEU 324	-2.607 -4.837 19.889 1.00 15.92
	ATOM	1260 CD1 LEU 324	-2.602 -3.547 20.692 1.00 15.92
	ATOM	1261 CD2 LEU 324	-3.182 -4.598 18.511 1.00 15.92
	ATOM	1262 C LEU 324	-1.393 -6.924 21.707 1.00 13.48
	ATOM	1263 O LEU 324	-1.896 -6.678 22.802 1.00 15.92
10	ATOM	1264 N MET 325	-1.593 -8.074 21.072 1.00 11.47
	ATOM	1265 CA MET 325	-2.458 -9.111 21.631 1.00 11.47
	ATOM	1266 CB MET 325	-2.959 -10.043 20.520 1.00 22.90
	ATOM	1267 CG MET 325	-3.689 -9.347 19.375 1.00 22.90
	ATOM	1268 SD MET 325	-5.052 -8.287 19.908 1.00 22.90
15	ATOM	1269 CE MET 325	-6.284 -9.475 20.353 1.00 22.90
	ATOM	1270 C MET 325	-1.814 -9.932 22.752 1.00 11.47
	ATOM	1271 O MET 325	-1.899 -11.160 22.758 1.00 22.90
	ATOM	1272 N SER 326	-1.193 -9.256 23.711 1.00 30.07
	ATOM	1273 CA SER 326	-0.543 -9.936 24.826 1.00 30.07
20	ATOM	1274 CB SER 326	0.723 -9.175 25.239 1.00 32.79
	ATOM	1275 OG SER 326	1.283 -9.699 26.433 1.00 32.79
	ATOM	1276 C SER 326	-1.492 -10.061 26.014 1.00 30.07
	ATOM	1277 O SER 326	-2.343 -9.198 26.235 1.00 32.79
	ATOM	1278 N THR 327	-1.347 -11.143 26.773 1.00 29.08
25	ATOM	1279 CA THR 327	-2.179 -11.368 27.948 1.00 29.08
	ATOM	1280 CB THR 327	-2.705 -12.817 27.998 1.00 36.96
	ATOM	1281 OG1 THR 327	-1.612 -13.734 27.856 1.00 36.96
	ATOM	1282 CG2 THR 327	-3.716 -13.055 26.890 1.00 36.96
20	ATOM	1283 C THR 327	-1.426 -11.049 29.239 1.00 29.08
30	ATOM	1284 O THR 327	-1.930 -11.295 30.333 1.00 36.96
	ATOM	1285 N ASP 328	-0.214 -10.513 29.111 1.00 38.93 0.596 -10.152 30.273 1.00 38.93
	ATOM	1286 CA ASP 328 1287 CB ASP 328	2.082 -10.089 29.899 1.00 85.70
	ATOM ATOM	1288 CG ASP 328	2.660 -11.451 29.556 1.00 85.70
35	ATOM	1289 OD1 ASP 328	3.388 -11.554 28.542 1.00 85.70
33	ATOM	1290 OD2 ASP 328	2.393 -12.418 30.303 1.00 85.70
	ATOM	1291 C ASP 328	0.148 -8.810 30.845 1.00 38.93
		1292 O ASP 328	0.962 -7.911 31.061 1.00 85.70
		1293 N ARG 329	-1.154 -8.673 31.070 1.00 28.95
40	ATOM		-1.716 -7.445 31.608 1.00 28.95
40	ATOM	1295 CB ARG 329	-2.390 -6.612 30.509 1.00 38.88
	ATOM	1296 CG ARG 329	-1.449 -5.887 29.554 1.00 38.88
	ATOM		-1.107 -6.739 28.347 1.00 38.88
	ATOM		-0.322 -6.005 27.356 1.00 38.88
45	ATOM	1299 CZ ARG 329	1.006 -5.936 27.351 1.00 38.88
73	ATOM	1300 NH1 ARG 329	1.713 -6.552 28.290 1.00 38.88
	ATOM	1301 NH2 ARG 329	1.631 -5.270 26.391 1.00 38.88
	ATOM	1302 C ARG 329	-2.745 -7.790 32.672 1.00 28.95
		1202 C ARG 327	2 270 0 000 22 606 1 00 28 88

ATOM 1303 O ARG 329 -3.279 -8.898 32.696 1.00 38.88 ATOM 1304 N SER 330 -3.029 -6.829 33.542 1.00 42.07

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ATOM 1305 CA SER 330
                                -3.999 -7.025 34.607 1.00 42.07
     ATOM 1306 CB SER 330
                                -3.488 -6.399 35.899 1.00 37.35
     ATOM 1307 C SER 330
                               -5.340 -6.413 34.220 1.00 42.07
     ATOM 1308 O SER 330
                               -5.386 -5.382 33.550 1.00 37.35
     ATOM 1309 N GLY 331
                                -6.424 -7.085 34.598 1.00 26.57
                                -7.754 -6.572 34.318 1.00 26.57
     ATOM 1310 CA GLY 331
                                -8.404 -6.915 32.991 1.00 26.57
     ATOM 1311 C GLY 331
     ATOM 1312 O GLY 331
                                -9.462 -6.371 32.671 1.00 30.06
     ATOM 1313 N LEU 332
                               -7.797 -7.807 32.214 1.00 31.47
     ATOM 1314 CA LEU 332
                                -8.374 -8.189 30.928 1.00 31.47
10
     ATOM 1315 CB LEU 332
                                -7.351 -8.933 30.065 1.00 23.83
    ATOM 1316 CG LEU 332
                                -6.261 -8.076 29.425 1.00 23.83
                                 -5.296 -8.960 28.652 1.00 23.83
     ATOM 1317 CD1 LEU 332
     ATOM 1318 CD2 LEU 332
                                 -6.897 -7.041 28.509 1.00 23.83
15
     ATOM 1319 C LEU 332
                               -9.630 -9.039 31.091 1.00 31.47
     ATOM 1320 O LEU 332
                               -9.665 -9.969 31.895 1.00 23.83
     ATOM 1321 N LEU 333
                               -10.659 -8.702 30.321 1.00 27.66
                                -11.927 -9.422 30.351 1.00 27.66
     ATOM 1322 CA LEU 333
                                -13.072 -8.500 29.918 1.00 49.79
     ATOM 1323 CB LEU 333
                                -13.416 -7.312 30.820 1.00 49.79
20
     ATOM 1324 CG LEU 333
     ATOM 1325 CD1 LEU 333
                                -14.328 -6.339 30.083 1.00 49.79
     ATOM 1326 CD2 LEU 333
                                -14.072 -7.803 32.104 1.00 49.79
     ATOM 1327 C LEU 333
                               -11.904 -10.663 29.456 1.00 27.66
     ATOM 1328 O LEU 333
                               -12.117 -11.780 29.919 1.00 49.79
                               -11.616 -10.464 28.174 1.00 29.56
25
     ATOM 1329 N CYS 334
                                -11.583 -11.566 27.220 1.00 29.56
     ATOM 1330 CA CYS 334
                                -12.134 -11.106 25.865 1.00 47.01
     ATOM 1331 CB CYS 334
     ATOM 1332 SG CYS 334
                               -13.888 -10.657 25.883 1.00 47.01
                               -10.187 -12.161 27.050 1.00 29.56
     ATOM 1333 C CYS 334
     ATOM 1334 O CYS 334
                               -9.652 -12.202 25.942 1.00 47.01
30
     ATOM 1335 N VAL 335
                                -9.617 -12.655 28.147 1.00 30.69
    ATOM 1336 CA VAL 335
                                -8.280 -13.250 28.132 1.00 30.69
                                -7.913 -13.844 29.514 1.00 32.18
    ATOM 1337 CB VAL 335
     ATOM 1338 CG1 VAL 335
                                 -6.517 -14.456 29.480 1.00 32.18
35
    ATOM 1339 CG2 VAL 335
                                -7.988 -12.768 30.584 1.00 32.18
     ATOM 1340 C VAL 335
                                -8.120 -14.340 27.068 1.00 30.69
     ATOM 1341 O VAL 335
                                -7.149 -14.337 26.309 1.00 32.18
     ATOM 1342 N ASP 336
                               -9.079 -15.260 27.012 1.00 30.13
     ATOM 1343 CA ASP 336
                                -9.040 -16.360 26.052 1.00 30.13
                               -10.218 -17.311 26.284 1.00 63.22
40
     ATOM 1344 CB ASP 336
    ATOM 1345 CG ASP 336
                                -10.178 -18.528 25.370 1.00 63.22
    ATOM 1346 OD1 ASP 336
                                -11.119 -18.700 24.565 1.00 63.22
    ATOM 1347 OD2 ASP 336
                                 -9.205 -19.311 25.452 1.00 63.22
                               -9.012 -15.903 24.594 1.00 30.13
     ATOM 1348 C ASP 336
                               -8.156 -16.339 23.823 1.00 63.22
45
    ATOM 1349 O ASP 336
                               -9.944 -15.027 24.223 1.00 26.63
    ATOM 1350 N LYS 337
    ATOM 1351 CA LYS 337
                               -10.024 -14.515 22.856 1.00 26.63
    ATOM 1352 CB LYS 337
                               -11.172 -13.516 22.729 1.00 21.38
    ATOM 1353 C LYS 337
                               -8.706 -13.865 22.438 1.00 26.63
     ATOM 1354 O LYS 337
                               -8.204 -14.110 21.338 1.00 21.38
50
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	ATOM	1355 N ILE 338	-8.141 -13.060 23.334 1.00 24.65
	ATOM	1356 CA ILE 338	-6.879 -12.376 23.078 1.00 24.65
	ATOM	1357 CB ILE 338	-6.543 -11.380 24.215 1.00 20.45
	ATOM	1358 CG2 ILE 338	-5.198 -10.719 23.966 1.00 20.45
5	ATOM	1359 CG1 ILE 338	-7.632 -10.308 24.308 1.00 20.45
	ATOM	1360 CD1 ILE 338	-7.479 -9.374 25.486 1.00 20.45
	ATOM	1361 C ILE 338	-5.744 -13.388 22.911 1.00 24.65
	ATOM	1362 O ILE 338	-4.948 -13.288 21.974 1.00 20.45
	ATOM	1363 N GLU 339	-5.700 -14.383 23.795 1.00 35.34
10	ATOM	1364 CA GLU 339	-4.673 -15.422 23.745 1.00 35.34
	ATOM	1365 CB GLU 339	-4.836 -16.388 24.916 1.00 29.51
	ATOM	1366 C GLU 339	-4.744 -16.180 22.421 1.00 35.34
	ATOM	1367 O GLU 339	-3.720 -16.421 21.777 1.00 29.51
	ATOM	1368 N LYS 340	-5.959 -16.536 22.009 1.00 24.19
15	ATOM	1369 CA LYS 340	-6.168 -17.256 20.755 1.00 24.19
	ATOM	1370 CB LYS 340	-7.627 -17.671 20.624 1.00 23.97
	ATOM	1371 C LYS 340	-5.754 -16.377 19.576 1.00 24.19
	ATOM	1372 O LYS 340	-5.197 -16.860 18.586 1.00 23.97
	ATOM	1373 N SER 341	-6.000 -15.079 19.708 1.00 16.85
20	ATOM	1374 CA SER 341	-5.651 -14.115 18.676 1.00 16.85
	ATOM	1375 CB SER 341	-6.223 -12.744 19.033 1.00 26.59
	ATOM	1376 OG SER 341	-5.852 -11.765 18.080 1.00 26.59
	ATOM	1377 C SER 341	-4.137 -14.026 18.500 1.00 16.85
	ATOM	1378 O SER 341	-3.638 -14.042 17.374 1.00 26.59
25	ATOM	1379 N GLN 342	-3.406 -13.932 19.608 1.00 17.35
	ATOM	1380 CA GLN 342	-1.952 -13.845 19.537 1.00 17.35
	ATOM	1381 CB GLN 342	-1.337 -13.597 20.913 1.00 30.07
	ATOM	1382 CG GLN 342	0.140 -13.245 20.832 1.00 30.07
	ATOM	1383 CD GLN 342	0.811 -13.196 22.182 1.00 30.07
30	ATOM	1384 OE1 GLN 342	0.884 -14.201 22.884 1.00 30.07
	ATOM	1385 NE2 GLN 342	1.318 -12.030 22.548 1.00 30.07
	ATOM	1386 C GLN 342	-1.368 -15.118 18.944 1.00 17.35
	ATOM	1387 O GLN 342	-0.405 -15.066 18.178 1.00 30.07
	ATOM	1388 N GLU 343	-1.949 -16.260 19.303 1.00 18.35
35	ATOM	1389 CA GLU 343	-1.489 -17.546 18.791 1.00 18.35
	ATOM	1390 CB GLU 343	-2.308 -18.676 19.394 1.00 16.98
	ATOM	1391 C GLU 343	-1.603 -17.560 17.267 1.00 18.35
	ATOM	1392 O GLU 343	-0.699 -18.026 16.568 1.00 16.98
	ATOM	1393 N ALA 344	-2.706 -17.017 16.761 1.00 14.83
40	ATOM	1394 CA ALA 344	-2.946 -16.948 15.324 1.00 14.83
	ATOM	1395 CB ALA 344	-4.327 -16.376 15.049 1.00 19.42
	ATOM	1396 C ALA 344	-1.872 -16.102 14.640 1.00 14.83
	ATOM	1397 O ALA 344	-1.311 -16.507 13.619 1.00 19.42
	ATOM	1398 N TYR 345	-1.586 -14.934 15.211 1.00 13.10
45	ATOM	1399 CA TYR 345	-0.569 -14.041 14.665 1.00 13.10
	ATOM	1400 CB TYR 345	-0.573 -12.697 15.393 1.00 2.00
	ATOM	1401 CG TYR 345	-1.670 -11.767 14.938 1.00 2.00
	ATOM	1402 CD1 TYR 345	-2.707 -11.409 15.794 1.00 2.00
_	ATOM	1403 CE1 TYR 345	-3.722 -10.562 15.377 1.00 2.00
50	ATOM	1404 CD2 TYR 345	-1.674 -11.248 13.647 1.00 2.00

			10 200 12 010 1 00 2 00
	ATOM	1405 CE2 TYR 345	-2.683 -10.398 13.219 1.00 2.00
	ATOM	1406 CZ TYR 345	-3.706 -10.061 14.087 1.00 2.00
	ATOM	1407 OH TYR 345	-4.722 -9.233 13.669 1.00 2.00
	ATOM	1408 C TYR 345	0.818 -14.666 14.732 1.00 13.10
5	ATOM	1409 O TYR 345	1.614 -14.504 13.811 1.00 2.00
	ATOM	1410 N LEU 346	1.101 -15.387 15.813 1.00 12.59
	ATOM	1411 CA LEU 346	2.396 -16.041 15.976 1.00 12.59
	ATOM	1412 CB LEU 346	2.498 -16.715 17.347 1.00 22.61
	ATOM	1413 CG LEU 346	2.899 -15.799 18.504 1.00 22.61
10	ATOM	1414 CD1 LEU 346	2.717 -16.511 19.830 1.00 22.61
	ATOM	1415 CD2 LEU 346	4.341 -15.357 18.324 1.00 22.61
	ATOM	1416 C LEU 346	2.629 -17.057 14.865 1.00 12.59
	ATOM	1417 O LEU 346	3.706 -17.099 14.272 1.00 22.61
	ATOM	1418 N LEU 347	1.612 -17.862 14.574 1.00 18.42
15	ATOM	1419 CA LEU 347	1.706 -18.863 13.517 1.00 18.42
	ATOM	1420 CB LEU 347	0.471 -19.762 13.512 1.00 23.56
	ATOM	1421 CG LEU 347	0.509 -20.965 14.456 1.00 23.56
	ATOM	1422 CD1 LEU 347	-0.819 -21.702 14.398 1.00 23.56
	ATOM	1423 CD2 LEU 347	1.659 -21.890 14.068 1.00 23.56
20	ATOM	1424 C LEU 347	1.870 -18.201 12.154 1.00 18.42
20	ATOM	1425 O LEU 347	2.672 -18.651 11.330 1.00 23.56
	ATOM	1426 N ALA 348	1.099 -17.144 11.917 1.00 12.49
	ATOM	1427 CA ALA 348	1.157 -16.403 10.663 1.00 12.49
	ATOM	1428 CB ALA 348	0.098 -15.302 10.654 1.00 14.77
25	ATOM	1429 C ALA 348	2.545 -15.798 10.504 1.00 12.49
23	ATOM	1430 O ALA 348	3.154 -15.874 9.436 1.00 14.77
	ATOM	1431 N PHE 349	3.048 -15.246 11.602 1.00 15.52
	ATOM	1432 CA PHE 349	4.357 -14.613 11.664 1.00 15.52
	ATOM	1433 CB PHE 349	4.566 -14.049 13.076 1.00 14.41
30	ATOM	1434 CG PHE 349	5.714 -13.085 13.203 1.00 14.41
50	ATOM	1435 CD1 PHE 349	6.473 -12.712 12.099 1.00 14.41
	ATOM	1436 CD2 PHE 349	6.027 -12.540 14.443 1.00 14.41
	ATOM	1437 CE1 PHE 349	7.523 -11.813 12.230 1.00 14.41
	ATOM	1438 CE2 PHE 349	7.075 -11.640 14.584 1.00 14.41
35	ATOM	1439 CZ PHE 349	7.825 -11.275 13.475 1.00 14.41
33	ATOM	1440 C PHE 349	5.444 -15.633 11.324 1.00 15.52
	ATOM	1441 O PHE 349	6.252 -15.413 10.422 1.00 14.41
	ATOM	1441 O FHE 349 1442 N GLU 350	5.439 -16.760 12.026 1.00 13.20
		1442 N GLU 330 1443 CA GLU 350	6.424 -17.811 11.801 1.00 13.20
40	ATOM		
40	ATOM	1444 CB GLU 350	6.152 -18.995 12.734 1.00 33.43 7.068 -20.193 12.519 1.00 33.43
	ATOM	1445 CG GLU 350	6.786 -21.331 13.482 1.00 33.43
	ATOM	1446 CD GLU 350	
	ATOM	1447 OE1 GLU 350	7.746 -22.035 13.857 1.00 33.43
4.5	ATOM	1448 OE2 GLU 350	5.611 -21.525 13.865 1.00 33.43
45	ATOM	1449 C GLU 350	6.409 -18.283 10.352 1.00 13.20
	ATOM	1450 O GLU 350	7.449 -18.355 9.694 1.00 33.43
	ATOM	1451 N HIS 351	5.217 -18.573 9.850 1.00 19.10
	ATOM	1452 CA HIS 351	5.062 -19.051 8.485 1.00 19.10
	ATOM	1453 CB HIS 351	3.632 -19.536 8.256 1.00 18.97
50	ATOM	1454 CG HIS 351	3.249 -20.700 9.117 1.00 18.97

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3.987 -21.474 9.948 1.00 18.97
     ATOM 1455 CD2 HIS 351
     ATOM 1456 ND1 HIS 351
                                1.960 -21.180 9.194 1.00 18.97
                                1.918 -22.195 10.039 1.00 18.97
     ATOM 1457 CE1 HIS 351
                                3.134 -22.394 10.509 1.00 18.97
     ATOM 1458 NE2 HIS 351
                               5.477 -18.011 7.449 1.00 19.10
     ATOM 1459 C HIS 351
                               5.955 -18.366 6.371 1.00 18.97
     ATOM 1460 O HIS 351
                                5.304 -16.732 7.767 1.00 9.38
     ATOM 1461 N TYR 352
                                5.711 -15.683 6.843 1.00 9.38
     ATOM 1462 CA TYR 352
                                 5.168 -14.317 7.257 1.00 16.06
     ATOM 1463 CB TYR 352
                                 5.539 -13.238 6.268 1.00 16.06
     ATOM 1464 CG TYR 352
10
                                 4.939 -13.190 5.008 1.00 16.06
     ATOM 1465 CD1 TYR 352
                                 5.321 -12.242 4.060 1.00 16.06
     ATOM 1466 CE1 TYR 352
                                 6.531 -12.303 6.562 1.00 16.06
     ATOM 1467 CD2 TYR 352
     ATOM 1468 CE2 TYR 352
                                 6.923 -11.349 5.620 1.00 16.06
     ATOM 1469 CZ TYR 352
                                6.313 -11.326 4.371 1.00 16.06
15
                                 6.710 -10.401 3.431 1.00 16.06
     ATOM 1470 OH TYR 352
                                7.234 -15.639 6.812 1.00 9.38
     ATOM 1471 C TYR 352
     ATOM 1472 O TYR 352
                                7.838 -15.475 5.751 1.00 16.06
                                7.851 -15.789 7.980 1.00 15.38
     ATOM 1473 N VAL 353
20
     ATOM 1474 CA VAL 353
                                 9.305 -15.790 8.087 1.00 15.38
                                 9.761 -15.945 9.558 1.00 18.40
     ATOM 1475 CB VAL 353
     ATOM 1476 CG1 VAL 353
                                 11.262 -16.163 9.633 1.00 18.40
     ATOM 1477 CG2 VAL 353
                                 9.384 -14.703 10.349 1.00 18.40
     ATOM 1478 C VAL 353
                                9.853 -16.938 7.237 1.00 15.38
     ATOM 1479 O VAL 353
                                10.850 -16.773 6.525 1.00 18.40
25
     ATOM 1480 N ASN 354
                                9.183 -18.086 7.298 1.00 14.74
     ATOM 1481 CA ASN 354
                                 9.578 -19.259 6.521 1.00 14.74
     ATOM 1482 CB ASN 354
                                 8.640 -20.435 6.799 1.00 19.97
     ATOM 1483 CG ASN 354
                                 8.832 -21.020 8.180 1.00 19.97
     ATOM 1484 OD1 ASN 354
                                 9.879 - 20.848 8.799 1.00 19.97
30
     ATOM 1485 ND2 ASN 354
                                 7.826 -21.734 8.664 1.00 19.97
     ATOM 1486 C ASN 354
                                9.550 -18.939 5.034 1.00 14.74
     ATOM 1487 O ASN 354
                                10.452 -19.319 4.290 1.00 19.97
     ATOM 1488 N HIS 355
                               8.507 -18.230 4.613 1.00 13.03
                                8.329 -17.837 3.220 1.00 13.03
     ATOM 1489 CA HIS 355
35
     ATOM 1490 CB HIS 355
                                6.960 -17.164 3.042 1.00 24.39
                                6.753 -16.541 1.695 1.00 24.39
     ATOM 1491 CG HIS 355
     ATOM 1492 CD2 HIS 355
                                7.195 -15.370 1.176 1.00 24.39
                                ATOM 1493 ND1 HIS 355
                                6.005 -16.368 -0.372 1.00 24.39
     ATOM 1494 CE1 HIS 355
40
                                6.720 -15.289 -0.107 1.00 24.39
     ATOM 1495 NE2 HIS 355
                               9.434 -16.894 2.758 1.00 13.03
     ATOM 1496 C HIS 355
                               9.834 -16.920 1.595 1.00 24.39
     ATOM 1497 O HIS 355
                                9.878 -16.027 3.660 1.00 19.55
     ATOM 1498 N ARG 356
                                10.920 - 15.054 3.358 1.00 19.55
     ATOM 1499 CA ARG 356
45
                                 10.970 -14.001 4.460 1.00 22.01
     ATOM 1500 CB ARG 356
                                 9.772 -13.081 4.454 1.00 22.01
     ATOM 1501 CG ARG 356
     ATOM 1502 CD ARG 356
                                 10.097 -11.784 3.750 1.00 22.01
                                10.932 - 10.934 4.592 1.00 22.01
     ATOM 1503 NE ARG 356
                                11.822 -10.059 4.137 1.00 22.01
     ATOM 1504 CZ ARG 356
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12.010 -9.907 2.833 1.00 22.01
    ATOM 1505 NH1 ARG 356
                                 12.519 -9.325 4.992 1.00 22.01
    ATOM 1506 NH2 ARG 356
                                12.297 -15.675 3.158 1.00 19.55
    ATOM 1507 C ARG 356
                                13.127 -15.126 2.434 1.00 22.01
    ATOM 1508 O ARG 356
    ATOM 1509 N LYS 357
                               12.547 -16.788 3.841 1.00 23.18
5
                                13.815 -17.504 3.739 1.00 23.18
    ATOM 1510 CA LYS 357
                                13.879 - 18.273 2.415 1.00 42.91
    ATOM 1511 CB LYS 357
                                12.750 -19.277 2.274 1.00 42.91
    ATOM 1512 CG LYS 357
                                12.773 -20.021 0.960 1.00 42.91
    ATOM 1513 CD LYS 357
                                11.619 -21.011 0.913 1.00 42.91
    ATOM 1514 CE LYS 357
10
                                11.629 -21.845 -0.316 1.00 42.91
    ATOM 1515 NZ LYS 357
                               15.047 -16.619 3.918 1.00 23.18
    ATOM 1516 C LYS 357
                               15.816 -16.396 2.982 1.00 42.91
    ATOM 1517 O LYS 357
                               15.228 -16.122 5.137 1.00 32.39
    ATOM 1518 N HIS 358
                                16.367 -15.272 5.460 1.00 32.39
    ATOM 1519 CA HIS 358
15
                                16.181 -14.626 6.835 1.00 26.77
    ATOM 1520 CB HIS 358
                                15.232 -13.468 6.841 1.00 26.77
    ATOM 1521 CG HIS 358
                                15.452 -12.138 6.709 1.00 26.77
    ATOM 1522 CD2 HIS 358
                                13.875 -13.615 7.028 1.00 26.77
     ATOM 1523 ND1 HIS 358
                                13.300 -12.426 7.012 1.00 26.77
20
    ATOM 1524 CE1 HIS 358
                                14.234 -11.513 6.821 1.00 26.77
     ATOM 1525 NE2 HIS 358
     ATOM 1526 C HIS 358
                               17.633 -16.115 5.480 1.00 32.39
                               17.618 -17.248 5.961 1.00 26.77
     ATOM 1527 O HIS 358
                                18.728 -15.561 4.972 1.00 41.97
     ATOM 1528 N ASN 359
                                20.000 -16.273 4.959 1.00 41.97
     ATOM 1529 CA ASN 359
25
                                20.909 -15.716 3.863 1.00 46.84
     ATOM 1530 CB ASN 359
                                20.663 -16.134 6.331 1.00 41.97
     ATOM 1531 C ASN 359
     ATOM 1532 O ASN 359
                                21.821 -15.731 6.436 1.00 46.84
                               19.908 -16.450 7.379 1.00 35.72
     ATOM 1533 N ILE 360
                                20.394 -16.359 8.753 1.00 35.72
     ATOM 1534 CA ILE 360
30
     ATOM 1535 CB ILE 360
                                19.819 - 15.113 9.480 1.00 36.14
     ATOM 1536 CG2 ILE 360
                                20.327 -15.050 10.918 1.00 36.14
     ATOM 1537 CG1 ILE 360
                                20.204 -13.833 8.734 1.00 36.14
     ATOM 1538 CD1 ILE 360
                                19.526 -12.591 9.265 1.00 36.14
     ATOM 1539 C ILE 360
                               19.935 -17.611 9.493 1.00 35.72
35
     ATOM 1540 O ILE 360
                               18.748 - 17.953 9.479 1.00 36.14
                                20.877 -18.338 10.109 1.00 31.56
     ATOM 1541 N PRO 361
                                22.334 -18.114 10.100 1.00 33.50
     ATOM 1542 CD PRO 361
                                20.532 -19.556 10.847 1.00 31.56
     ATOM 1543 CA PRO 361
                                21.901 -20.163 11.161 1.00 33.50
     ATOM 1544 CB PRO 361
40
                                22.801 -18.967 11.249 1.00 33.50
     ATOM 1545 CG PRO 361
                                19.743 -19.256 12.121 1.00 31.56
     ATOM 1546 C PRO 361
                                20.080 -18.338 12.867 1.00 33.50
     ATOM 1547 O PRO 361
                               18.688 -20.034 12.355 1.00 18.84
     ATOM 1548 N HIS 362
                                17.840 -19.887 13.541 1.00 18.84
45
     ATOM 1549 CA HIS 362
                                18.656 -20.151 14.812 1.00 31.38
     ATOM 1550 CB HIS 362
     ATOM 1551 CG HIS 362
                                19.540 -21.357 14.731 1.00 31.38
                                19.250 -22.667 14.537 1.00 31.38
     ATOM 1552 CD2 HIS 362
                                20.910 -21.286 14.860 1.00 31.38
     ATOM 1553 ND1 HIS 362
                                21.427 -22.497 14.754 1.00 31.38
     ATOM 1554 CE1 HIS 362
50
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	ATOM	1555 NE2 HIS 362	20.439 -23.353 14.558 1.00 31.38
	ATOM	1556 C HIS 362	17.189 -18.506 13.628 1.00 18.84
	ATOM	1557 O HIS 362	16.980 -17.979 14.723 1.00 31.38
	ATOM	1558 N PHE 363	16,825 -17.950 12.476 1.00 18.69
5	ATOM	1559 CA PHE 363	16.209 -16.630 12.408 1.00 18.69
	ATOM	1560 CB PHE 363	15,825 -16.302 10.962 1.00 19.25
	ATOM	1561 CG PHE 363	15.339 -14.894 10.765 1.00 19.25
	ATOM	1562 CD1 PHE 363	16.239 -13.862 10.530 1.00 19.25
	ATOM	1563 CD2 PHE 363	13.981 -14.598 10.819 1.00 19.25
10	ATOM	1564 CE1 PHE 363	15.794 -12.556 10.351 1.00 19.25
	ATOM	1565 CE2 PHE 363	13.527 -13.296 10.642 1.00 19.25
	ATOM	1566 CZ PHE 363	14.435 -12.273 10.407 1.00 19.25
	ATOM	1567 C PHE 363	14.995 -16.461 13.323 1.00 18.69
	ATOM	1568 O PHE 363	14.955 -15.540 14.138 1.00 19.25
15	ATOM	1569 N TRP 364	14.016 -17.351 13.191 1.00 16.46
	ATOM	1570 CA TRP 364	12.797 -17.280 13.995 1.00 16.46
	ATOM	1571 CB TRP 364	11.882 -18.482 13.706 1.00 17.81
	ATOM	1572 CG TRP 364	10.588 -18.488 14.481 1.00 17.81
	ATOM	1573 CD2 TRP 364	9.586 -17.458 14.504 1.00 17.81
20	ATOM	1574 CE2 TRP 364	8.547 -17.905 15.350 1.00 17.81
	ATOM	1575 CE3 TRP 364	9.467 -16.202 13.894 1.00 17.81
	ATOM	1576 CD1 TRP 364	10.126 -19.486 15.290 1.00 17.81
	ATOM	1577 NE1 TRP 364	8.902 -19.144 15.814 1.00 17.81
	ATOM	1578 CZ2 TRP 364	7.403 -17.142 15.602 1.00 17.81
25	ATOM	1579 CZ3 TRP 364	8.329 -15.444 14.145 1.00 17.81
	ATOM	1580 CH2 TRP 364	7.312 -15.919 14.992 1.00 17.81
	ATOM	1581 C TRP 364	13.046 -17.114 15.500 1.00 16.46
	ATOM	1582 O TRP 364	12.595 -16.133 16.087 1.00 17.81
20	ATOM	1583 N PRO 365	13.779 -18.051 16.137 1.00 18.31 14.342 -19.314 15.625 1.00 25.61
30	ATOM	1584 CD PRO 365	14.342 -19.314 13.623 1.00 23.61
	ATOM	1585 CA PRO 365	14.038 -17.920 17.377 1.00 18.31
	ATOM	1586 CB PRO 365 1587 CG PRO 365	14.500 -20.130 16.882 1.00 25.61
	ATOM ATOM	1587 CG PRO 365 1588 C PRO 365	14.732 -16.606 17.933 1.00 18.31
35	ATOM	1589 O PRO 365	14.387 -15.963 18.926 1.00 25.61
33	ATOM	1590 N LYS 366	15.699 -16.207 17.112 1.00 25.16
	ATOM	1591 CA LYS 366	16.439 -14.968 17.338 1.00 25.16
	ATOM	1591 CA LTS 366	17.537 -14.805 16.289 1.00 40.51
	ATOM	1592 CB LTS 366	18.679 -15.792 16.417 1.00 40.51
40	ATOM	1594 CD LYS 366	19.664 -15.607 15.278 1.00 40.51
40	ATOM	1595 CE LYS 366	20.884 -16.492 15.440 1.00 40.51
	ATOM	1596 NZ LYS 366	21.800 -16.360 14.275 1.00 40.51
	ATOM	1597 C LYS 366	15.521 -13.747 17.317 1.00 25.16
	ATOM	1598 O LYS 366	15.593 -12.893 18.202 1.00 40.51
45	ATOM	1599 N LEU 367	14.661 -13.666 16.307 1.00 25.30
	ATOM	1600 CA LEU 367	13.729 -12.551 16.184 1.00 25.30
	ATOM	1601 CB LEU 367	12.989 -12.620 14.845 1.00 27.80
	ATOM	1602 CG LEU 367	11.964 -11.519 14.561 1.00 27.80
	ATOM	1603 CD1 LEU 367	12.621 -10.147 14.679 1.00 27.80
50	ATOM	1604 CD2 LEU 367	11.367 -11.724 13.175 1.00 27.80

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ATOM 1605 C LEU 367
                               12.730 -12.596 17.332 1.00 25.30
     ATOM 1606 O LEU 367
                               12.337 -11.563 17.877 1.00 27.80
                                12.345 -13.807 17.712 1.00 26.12
     ATOM 1607 N LEU 368
     ATOM 1608 CA LEU 368
                                11.396 -14.019 18.793 1.00 26.12
                                11.105 -15.515 18.919 1.00 33.27
    ATOM 1609 CB LEU 368
                                 9.696 -15.976 19.289 1.00 33.27
     ATOM 1610 CG LEU 368
                                 8.640 -15.182 18.529 1.00 33.27
    ATOM 1611 CD1 LEU 368
                                 9.582 -17.460 18.976 1.00 33.27
     ATOM 1612 CD2 LEU 368
                               11.973 -13.466 20.096 1.00 26.12
     ATOM 1613 C LEU 368
                                11.249 -12.920 20.930 1.00 33.27
     ATOM 1614 O LEU 368
10
                                13.289 -13.571 20.244 1.00 24.39
    ATOM 1615 N MET 369
    ATOM 1616 CA MET 369
                                13.971 -13.076 21.432 1.00 24.39
                                 15.382 -13.656 21.511 1.00 47.44
    ATOM 1617 CB MET 369
     ATOM 1618 CG MET 369
                                 15.407 - 15.096 22.009 1.00 47.44
    ATOM 1619 SD MET 369
                                 16.850 -16.029 21.464 1.00 47.44
15
     ATOM 1620 CE MET 369
                                 18.186 -15.114 22.246 1.00 47.44
     ATOM 1621 C MET 369
                                13.996 -11.552 21.491 1.00 24.39
                                14.212 -10.971 22.557 1.00 47.44
     ATOM 1622 O MET 369
                                13.749 -10.904 20.354 1.00 27.31
     ATOM 1623 N LYS 370
                                13.713 -9.445 20.297 1.00 27.31
20
    ATOM 1624 CA LYS 370
                                13.739 -8.951 18.847 1.00 28.20
     ATOM 1625 CB LYS 370
     ATOM 1626 CG LYS 370
                                15.004 -9.312 18.090 1.00 28.20
                                16.231 -8.810 18.824 1.00 28.20
     ATOM 1627 CD LYS 370
                                17.512 -9.244 18.142 1.00 28.20
     ATOM 1628 CE LYS 370
                                18.696 -8.851 18.952 1.00 28.20
25
     ATOM 1629 NZ LYS 370
                               12.453 -8.945 21.002 1.00 27.31
     ATOM 1630 C LYS 370
     ATOM 1631 O LYS 370
                                12.424 -7.835 21.535 1.00 28.20
     ATOM 1632 N VAL 371
                                11.413 -9.776 21.009 1.00 26.41
     ATOM 1633 CA VAL 371
                                 10.157 -9.432 21.668 1.00 26.41
                                 9.109 -10.561 21.512 1.00 25.61
30
     ATOM 1634 CB VAL 371
     ATOM 1635 CG1 VAL 371
                                 7.825 -10.205 22.245 1.00 25.61
     ATOM 1636 CG2 VAL 371
                                 8.819 -10.805 20.044 1.00 25.61
     ATOM 1637 C VAL 371
                                10.450 -9.205 23.151 1.00 26.41
     ATOM 1638 O VAL 371
                                9.962 -8.248 23.752 1.00 25.61
     ATOM 1639 N THR 372
                                11.294 -10.065 23.713 1.00 26.28
35
     ATOM 1640 CA THR 372
                                11.683 -9.972 25.116 1.00 26.28
     ATOM 1641 CB THR 372
                                 12.656 -11.109 25.500 1.00 28.14
     ATOM 1642 OG1 THR 372
                                 12.025 -12.377 25.275 1.00 28.14
     ATOM 1643 CG2 THR 372
                                 13.055 -11.001 26.965 1.00 28.14
                                12.358 -8.624 25.372 1.00 26.28
     ATOM 1644 C THR 372
40
     ATOM 1645 O THR 372
                                12.047 -7.937 26.350 1.00 28.14
                                13.269 -8.247 24.478 1.00 15.09
     ATOM 1646 N ASP 373
                                13.977 -6.979 24.588 1.00 15.09
     ATOM 1647 CA ASP 373
                                14.976 -6.822 23.435 1.00 37.94
     ATOM 1648 CB ASP 373
                                16.065 -7.893 23.445 1.00 37.94
     ATOM 1649 CG ASP 373
45
                                 16.248 -8.571 24.483 1.00 37.94
     ATOM 1650 OD1 ASP 373
                                 16.750 -8.052 22.410 1.00 37.94
     ATOM 1651 OD2 ASP 373
     ATOM 1652 C ASP 373
                               12.969 -5.833 24.577 1.00 15.09
                               13.040 -4.928 25.407 1.00 37.94
     ATOM 1653 O ASP 373
                                12.008 -5.901 23.659 1.00 17.04
     ATOM 1654 N LEU 374
50
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ATOM 1655 CA LEU 374
                                10.974 -4.880 23.549 1.00 17.04
     ATOM 1656 CB LEU 374
                                10.071 -5.155 22.344 1.00 20.58
     ATOM 1657 CG LEU 374
                                10.624 -4.720 20.985 1.00 20.58
                                 9.826 -5.352 19.862 1.00 20.58
     ATOM 1658 CD1 LEU 374
                                 10.599 -3.202 20.882 1.00 20.58
     ATOM 1659 CD2 LEU 374
                               10.145 -4.786 24.825 1.00 17.04
     ATOM 1660 C LEU 374
                                9.783 -3.688 25.256 1.00 20.58
     ATOM 1661 O LEU 374
                                9.850 -5.935 25.430 1.00 20.46
     ATOM 1662 N ARG 375
                                 9.080 -5.977 26.673 1.00 20.46
     ATOM 1663 CA ARG 375
                                 8.873 -7.422 27.140 1.00 55.89
10
     ATOM 1664 CB ARG 375
                                 8.180 -8.354 26.152 1.00 55.89
     ATOM 1665 CG ARG 375
                                 6.692 -8.084 26.027 1.00 55.89
     ATOM 1666 CD ARG 375
                                 5.943 -9.338 25.968 1.00 55.89
     ATOM 1667 NE ARG 375
     ATOM 1668 CZ ARG 375
                                5.054 -9.654 25.028 1.00 55.89
                                 4.782 -8.808 24.040 1.00 55.89
     ATOM 1669 NH1 ARG 375
15
     ATOM 1670 NH2 ARG 375
                                 4.438 -10.829 25.073 1.00 55.89
                                9.874 -5.221 27.735 1.00 20.46
     ATOM 1671 C ARG 375
                                9.328 -4.391 28.463 1.00 55.89
     ATOM 1672 O ARG 375
                                11.174 -5.502 27.794 1.00 20.10
     ATOM 1673 N MET 376
                                12.076 -4.863 28.744 1.00 20.10
20
     ATOM 1674 CA MET 376
                                13.493 -5.417 28.580 1.00 63.73
     ATOM 1675 CB MET 376
     ATOM 1676 CG MET 376
                                13.956 -6.310 29.722 1.00 63.73
     ATOM 1677 SD MET 376
                                14.494 -5.373 31.182 1.00 63.73
     ATOM 1678 CE MET 376
                                12.934 -5.151 32.087 1.00 63.73
                               12.081 -3.347 28.566 1.00 20.10
25
     ATOM 1679 C MET 376
                                11.973 -2.602 29.539 1.00 63.73
     ATOM 1680 O MET 376
     ATOM 1681 N ILE 377
                               12.194 -2.896 27.321 1.00 30.02
     ATOM 1682 CA ILE 377
                               12.198 -1.469 27.014 1.00 30.02
     ATOM 1683 CB ILE 377
                               12.329 -1.228 25.488 1.00 19.31
30
     ATOM 1684 CG2 ILE 377
                                12.088 0.242 25.152 1.00 19.31
     ATOM 1685 CG1 ILE 377
                                13.711 -1.685 25.011 1.00 19.31
                                13.906 -1.634 23.507 1.00 19.31
     ATOM 1686 CD1 ILE 377
     ATOM 1687 C ILE 377
                               10.915 -0.821 27.542 1.00 30.02
     ATOM 1688 O ILE 377
                               10.962 0.216 28.211 1.00 19.31
                                9.779 -1.455 27.266 1.00 21.85
     ATOM 1689 N GLY 378
35
     ATOM 1690 CA GLY 378
                                8.505 -0.936 27.729 1.00 21.85
     ATOM 1691 C GLY 378
                                8.459 -0.821 29.243 1.00 21.85
     ATOM 1692 O GLY 378
                                7.990 0.185 29.779 1.00 34.01
                                8.967 -1.842 29.928 1.00 31.30
     ATOM 1693 N ALA 379
                                 8.996 -1.870 31.388 1.00 31.30
40
     ATOM 1694 CA ALA 379
     ATOM 1695 CB ALA 379
                                 9.471 -3.231 31.880 1.00 30.06
     ATOM 1696 C ALA 379
                                9.895 -0.763 31.938 1.00 31.30
     ATOM 1697 O ALA 379
                                9.482 0.002 32.810 1.00 30.06
     ATOM 1698 N CYS 380
                               11.117 -0.677 31.418 1.00 28.61
     ATOM 1699 CA CYS 380
                                12.067 0.349 31.841 1.00 28.61
45
                                13.360 0.268 31.025 1.00 60.26
     ATOM 1700 CB CYS 380
     ATOM 1701 SG CYS 380
                                14.499 -1.067 31.470 1.00 60.26
     ATOM 1702 C CYS 380
                               11.449 1.730 31.658 1.00 28.61
                               11.516 2.573 32.554 1.00 60.26
     ATOM 1703 O CYS 380
                               10.840 1.957 30.498 1.00 30.42
50
     ATOM 1704 N HIS 381
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	ATOM	1705 CA HIS 381	10.212 3.243 30.216 1.00 30.42
	ATOM	1706 CB HIS 381	9.696 3.306 28.779 1.00 16.49
	ATOM	1707 CG HIS 381	8.942 4.562 28.472 1.00 16.49
	ATOM	1708 CD2 HIS 381	9.370 5.805 28.151 1.00 16.49
5	ATOM	1709 ND1 HIS 381	7.566 4.633 28.524 1.00 16.49
	ATOM	1710 CE1 HIS 381	7.180 5.866 28.251 1.00 16.49
	ATOM	1711 NE2 HIS 381	8.255 6.596 28.021 1.00 16.49
	ATOM	1712 C HIS 381	9.073 3.539 31.182 1.00 30.42
	ATOM	1713 O HIS 381	8.856 4.690 31.552 1.00 16.49
10	ATOM	1714 N ALA 382	8.330 2.506 31.564 1.00 22.89
	ATOM	1715 CA ALA 382	7.218 2.666 32.493 1.00 22.89
	ATOM	1716 CB ALA 382	6.520 1.336 32.708 1.00 34.50
	ATOM	1717 C ALA 382	7.738 3.213 33.819 1.00 22.89
	ATOM	1718 O ALA 382	7.219 4.200 34.343 1.00 34.50
15	ATOM	1719 N SER 383	8.789 2.586 34.336 1.00 26.39
	ATOM	1720 CA SER 383	9.400 3.006 35.591 1.00 26.39
	ATOM	1721 CB SER 383	10.510 2.030 35.985 1.00 52.94
	ATOM	1722 OG SER 383	10.015 0.702 36.046 1.00 52.94
	ATOM	1723 C SER 383	9.966 4.418 35.470 1.00 26.39
20	ATOM	1724 O SER 383	9.772 5.253 36.357 1.00 52.94
	ATOM	1725 N ARG 384	10.662 4.683 34.368 1.00 30.36
	ATOM	1726 CA ARG 384	11.249 5.995 34.134 1.00 30.36
	ATOM	1727 CB ARG 384	12.116 5.977 32.874 1.00 37.39
	ATOM	1728 CG ARG 384	12.601 7.344 32.431 1.00 37.39
25	ATOM	1729 CD ARG 384	14.070 7.321 32.060 1.00 37.39
	ATOM	1730 NE ARG 384	14.935 7.597 33.204 1.00 37.39
	ATOM	1731 CZ ARG 384	15.750 8.646 33.291 1.00 37.39
	ATOM	1732 NH1 ARG 384	15.824 9.529 32.303 1.00 37.39
	ATOM	1733 NH2 ARG 384	16.488 8.819 34.376 1.00 37.39
30	ATOM	1734 C ARG 384	10.169 7.067 34.030 1.00 30.36
	ATOM	1735 O ARG 384	10.301 8.144 34.616 1.00 37.39
	ATOM	1736 N PHE 385	9.078 6.749 33.338 1.00 24.47
	ATOM	1737 CA PHE 385	7.980 7.693 33.171 1.00 24.47
~ ~	ATOM	1738 CB PHE 385	6.859 7.092 32.319 1.00 28.70
35	ATOM	1739 CG PHE 385	5.710 8.036 32.075 1.00 28.70
	ATOM	1740 CD1 PHE 385	5.795 9.017 31.092 1.00 28.70 4.549 7.954 32.836 1.00 28.70
	ATOM	1741 CD2 PHE 385	
	ATOM	1742 CE1 PHE 385	4.740 9.903 30.874 1.00 28.70
40	ATOM	1743 CE2 PHE 385	3.491 8.835 32.624 1.00 28.70
40	ATOM	1744 CZ PHE 385	3.587 9.812 31.641 1.00 28.70
	ATOM	1745 C PHE 385	7.436 8.097 34.533 1.00 24.47
	ATOM	1746 O PHE 385	7.250 9.285 34.805 1.00 28.70 7.208 7.107 35.391 1.00 31.13
	ATOM	1747 N LEU 386	
4.5	ATOM	1748 CA LEU 386	
45	ATOM	1749 CB LEU 386 1750 C LEU 386	6.596 6.044 37.513 1.00 39.10 7.577 8.348 37.474 1.00 31.13
	ATOM		7.085 9.201 38.217 1.00 39.10
	ATOM ATOM	1751 O LEU 386 1752 N HIS 387	8.884 8.254 37.243 1.00 36.46
	ATOM	1752 N HIS 387	9.837 9.152 37.881 1.00 36.46
50		1754 CB HIS 387	
50	ATOM	1/34 CB HIS 30/	11.258 8.589 37.794 1.00 62.78

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11.459 7.338 38.590 1.00 62.78
    ATOM 1755 CG HIS 387
                               10.601 6.614 39.346 1.00 62.78
    ATOM 1756 CD2 HIS 387
                                12.675 6.689 38.663 1.00 62.78
    ATOM 1757 ND1 HIS 387
                               12.554 5.620 39.431 1.00 62.78
    ATOM 1758 CE1 HIS 387
                               11.309 5.550 39.856 1.00 62.78
    ATOM 1759 NE2 HIS 387
                               9.778 10.544 37.266 1.00 36.46
    ATOM 1760 C HIS 387
                               9.885 11.543 37.979 1.00 62.78
    ATOM 1761 O HIS 387
                               9.587 10.612 35.950 1.00 33.41
    ATOM 1762 N MET 388
    ATOM 1763 CA MET 388
ATOM 1764 CB MET 388
                                9.505 11.894 35.258 1.00 33.41
                                9.269 11.703 33.755 1.00 42.63
10
                                10.456 11.144 32.982 1.00 42.63
    ATOM 1765 CG MET 388
                                10.253 11.325 31.192 1.00 42.63
    ATOM 1766 SD MET 388
    ATOM 1767 CE MET 388
                                9.501 9.772 30.748 1.00 42.63
    ATOM 1768 C MET 388
                                8.385 12.746 35.849 1.00 33.41
    ATOM 1769 O MET 388
                                8.573 13.934 36.103 1.00 42.63
15
                               7.235 12.126 36.092 1.00 39.26
    ATOM 1770 N LYS 389
                                6.082 12.825 36.659 1.00 39.26
    ATOM 1771 CA LYS 389
                                4.867 11.900 36.719 1.00 52.87
    ATOM 1772 CB LYS 389
                                4.237 11.594 35.379 1.00 52.87
    ATOM 1773 CG LYS 389
20
    ATOM 1774 CD LYS 389
                                3.048 10.667 35.553 1.00 52.87
                                3.482 9.327 36.125 1.00 52.87
    ATOM 1775 CE LYS 389
                                2.335 8.407 36.326 1.00 52.87
    ATOM 1776 NZ LYS 389
    ATOM 1777 C LYS 389
                               6.363 13.360 38.056 1.00 39.26
    ATOM 1778 O LYS 389
                               5.837 14.404 38.452 1.00 52.87
    ATOM 1779 N VAL 390
                                7.156 12.614 38.818 1.00 44.18
25
                                7.508 13.016 40.172 1.00 44.18
    ATOM 1780 CA VAL 390
                                8.299 11.898 40.905 1.00 50.50
    ATOM 1781 CB VAL 390
    ATOM 1782 CG1 VAL 390
                                 8.718 12.362 42.293 1.00 50.50
    ATOM 1783 CG2 VAL 390
                                 7.455 10.640 41.012 1.00 50.50
    ATOM 1784 C VAL 390
                                8.352 14.288 40.145 1.00 44.18
30
                                8.144 15.198 40.948 1.00 50.50
    ATOM 1785 O VAL 390
                                9.261 14.368 39.179 1.00 38.64
    ATOM 1786 N GLU 391
                                10.161 15.509 39.056 1.00 38.64
    ATOM 1787 CA GLU 391
    ATOM 1788 CB GLU 391
                                11.483 15.060 38.424 1.00 64.18
    ATOM 1789 CG GLU 391
                                12.065 13.766 39.009 1.00 64.18
35
    ATOM 1790 CD GLU 391
                                12.662 13.922 40.405 1.00 64.18
                                12.190 14.773 41.192 1.00 64.18
    ATOM 1791 OE1 GLU 391
    ATOM 1792 OE2 GLU 391
                                13.611 13.173 40.721 1.00 64.18
    ATOM 1793 C GLU 391
                                9.623 16.737 38.314 1.00 38.64
    ATOM 1794 O GLU 391
                                9.656 17.850 38.849 1.00 64.18
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    ATOM 1795 N CYS 392
                                9.125 16.539 37.096 1.00 37.24
                                8.611 17.635 36.271 1.00 37.24
    ATOM 1796 CA CYS 392
                                8.879 17.345 34.784 1.00 30.64
    ATOM 1797 CB CYS 392
                                10.634 17.137 34.283 1.00 30.64
    ATOM 1798 SG CYS 392
    ATOM 1799 C CYS 392
                                7.110 17.882 36.496 1.00 37.24
45
                                6.403 17.011 37.006 1.00 30.64
    ATOM 1800 O CYS 392
                                6.625 19.107 36.199 1.00 40.56
    ATOM 1801 N PRO 393
     ATOM 1802 CD PRO 393
                                7.444 20.297 35.904 1.00 33.41
                                5.209 19.473 36.358 1.00 40.56
    ATOM 1803 CA PRO 393
                                5,253 21.001 36.404 1.00 33.41
    ATOM 1804 CB PRO 393
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	ATOM	1805 CG PRO 393	6.409 21.332 35.527 1.00 33.41
	ATOM	1806 C PRO 393	4.330 18.975 35.207 1.00 40.56
	ATOM	1807 O PRO 393	4.776 18.907 34.057 1.00 33.41
	ATOM	1808 N THR 394	3.067 18.691 35.516 1.00 41.91
5	ATOM	1809 CA THR 394	2.101 18.186 34.540 1.00 41.91
	ATOM	1810 CB THR 394	0.691 18.075 35.156 1.00 62.04
	ATOM	1811 OG1 THR 394	0.706 18.582 36.497 1.00 62.04
	ATOM	1812 CG2 THR 394	0.232 16.626 35.168 1.00 62.04
	ATOM	1813 C THR 394	1.995 18.984 33.242 1.00 41.91
10	ATOM	1814 O THR 394	1.758 18.411 32.181 1.00 62.04
	ATOM	1815 N GLU 395	2.191 20.297 33.327 1.00 43.92
	ATOM	1816 CA GLU 395	2.104 21.176 32.160 1.00 43.92
	ATOM	1817 CB GLU 395	2.313 22.626 32.585 1.00 34.22
	ATOM	1818 C GLU 395	3.071 20.814 31.031 1.00 43.92
15	ATOM	1819 O GLU 395	2.887 21.243 29.891 1.00 34.22
	ATOM	1820 N LEU 396	4.104 20.041 31.350 1.00 34.92
	ATOM	1821 CA LEU 396	5.096 19.634 30.359 1.00 34.92
	ATOM	1822 CB LEU 396	6.473 19.495 31.017 1.00 35.81
	ATOM	1823 CG LEU 396	7.074 20.747 31.662 1.00 35.81
20	ATOM	1824 CD1 LEU 396	8.427 20.410 32.263 1.00 35.81
	ATOM	1825 CD2 LEU 396	7.209 21.857 30.629 1.00 35.81
	ATOM	1826 C LEU 396	4.731 18.324 29.661 1.00 34.92
	ATOM	1827 O LEU 396	5.343 17.954 28.659 1.00 35.81
	ATOM	1828 N PHE 397	3.734 17.627 30.197 1.00 35.28
25	ATOM	1829 CA PHE 397	3.302 16.352 29.640 1.00 35.28
	ATOM	1830 CB PHE 397	3.059 15.341 30.764 1.00 27.13
	ATOM	1831 CG PHE 397	4.285 15.004 31.561 1.00 27.13
	ATOM	1832 CD1 PHE 397	4.700 15.824 32.604 1.00 27.13
	ATOM	1833 CD2 PHE 397	5.021 13.860 31.273 1.00 27.13
30	ATOM	1834 CE1 PHE 397	5.831 15.510 33.349 1.00 27.13
	ATOM	1835 CE2 PHE 397	6.155 13.537 32.013 1.00 27.13
	ATOM	1836 CZ PHE 397	6.561 14.364 33.052 1.00 27.13 2.027 16.474 28.812 1.00 35.28
	ATOM	1837 C PHE 397	
2.5	ATOM	1838 O PHE 397	
35	ATOM	1839 N PRO 398	2.102 16.164 27.505 1.00 26.41 3.305 15.850 26.713 1.00 19.32
	ATOM	1840 CD PRO 398	
	ATOM	1841 CA PRO 398	
	ATOM	1842 CB PRO 398	1.439 15.752 25.300 1.00 19.32 2.867 16.193 25.312 1.00 19.32
40	ATOM	1843 CG PRO 398	
40	ATOM	1844 C PRO 398 1845 O PRO 398	-0.157 15.313 27.206 1.00 26.41 0.160 14.232 27.710 1.00 19.32
	ATOM ATOM	1846 N PRO 399	-1.439 15.702 27.104 1.00 25.12
	ATOM	1847 CD PRO 399	-1.437 13.702 27.104 1.00 25.12
	ATOM	1848 CA PRO 399	-2.554 14.894 27.612 1.00 25.12
45	ATOM	1849 CB PRO 399	-3.777 15.594 27.022 1.00 24.32
43	ATOM	1850 CG PRO 399	-3.349 17.026 26.974 1.00 24.32
	ATOM	1851 C PRO 399	-2.502 13.416 27.222 1.00 25.12
	ATOM	1852 O PRO 399	-2.599 12.540 28.085 1.00 24.32
	ATOM	1853 N LEU 400	-2.322 13.139 25.933 1.00 23.10
50	ATOM	1854 CA LEU 400	-2.265 11.759 25.454 1.00 23.10
50	ATOM	1054 011 1110 400	2.203 11.707 20.707 1.00 25.10

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-2.230 11.720 23.923 1.00 22.35
    ATOM 1855 CB LEU 400
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    ATOM 1856 CG LEU 400
                                -3.792 9.765 23.792 1.00 22.35
    ATOM 1857 CD1 LEU 400
                                -2.523 10.494 21.763 1.00 22.35
    ATOM 1858 CD2 LEU 400
                              -1.066 11.012 26.032 1.00 23.10
    ATOM 1859 C LEU 400
    ATOM 1860 O LEU 400
                               -1.160 9.825 26.345 1.00 22.35
                               0.044 11.723 26.202 1.00 13.85
    ATOM 1861 N PHE 401
    ATOM 1862 CA PHE 401
                                1.269 11.150 26.755 1.00 13.85
                                2.374 12.213 26.753 1.00 26.97
    ATOM 1863 CB PHE 401
                                3.729 11.702 27.164 1.00 26.97
    ATOM 1864 CG PHE 401
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                                4.189 10.461 26.732 1.00 26.97
    ATOM 1865 CD1 PHE 401
                                4.561 12.481 27.963 1.00 26.97
    ATOM 1866 CD2 PHE 401
    ATOM 1867 CE1 PHE 401
                                5.459 10.005 27.091 1.00 26.97
                                5.830 12.035 28.327 1.00 26.97
    ATOM 1868 CE2 PHE 401
                                6.280 10.795 27.889 1.00 26.97
    ATOM 1869 CZ PHE 401
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    ATOM 1870 C PHE 401
                               0.993 10.659 28.179 1.00 13.85
    ATOM 1871 O PHE 401
                               1.393 9.558 28.555 1.00 26.97
    ATOM 1872 N LEU 402
                               0.274 11.473 28.947 1.00 25.21
    ATOM 1873 CA LEU 402
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                                -0.640 12.380 31.035 1.00 29.34
    ATOM 1874 CB LEU 402
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    ATOM 1875 CG LEU 402
                                0.334 13.411 31.600 1.00 29.34
                                -0.430 14.658 32.018 1.00 29.34
    ATOM 1876 CD1 LEU 402
                                1.090 12.814 32.775 1.00 29.34
    ATOM 1877 CD2 LEU 402
                               -1.109 10.025 30.425 1.00 25.21
    ATOM 1878 C LEU 402
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    ATOM 1879 O LEU 402
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                               -2.090 10.043 29.529 1.00 23.54
    ATOM 1880 N GLU 403
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    ATOM 1881 CA GLU 403
                                -4.274 9.482 28.562 1.00 63.22
    ATOM 1882 CB GLU 403
                                -5.469 8.531 28.506 1.00 63.22
    ATOM 1883 CG GLU 403
                                -6.530 8.952 27.498 1.00 63.22
    ATOM 1884 CD GLU 403
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                                -6.237 9.786 26.613 1.00 63.22
    ATOM 1885 OE1 GLU 403
                                -7.666 8.436 27.589 1.00 63.22
    ATOM 1886 OE2 GLU 403
                               -2.708 7.629 29.170 1.00 23.54
    ATOM 1887 C GLU 403
     ATOM 1888 O GLU 403
                               -3.210 6.656 29.735 1.00 63.22
                               -1.787 7.515 28.221 1.00 33.24
     ATOM 1889 N VAL 404
35
                                -1.297 6.213 27.782 1.00 33.24
    ATOM 1890 CA VAL 404
                                -0.621 6.314 26.390 1.00 30.71
    ATOM 1891 CB VAL 404
                                -0.097 4.957 25.947 1.00 30.71
    ATOM 1892 CG1 VAL 404
                                -1.611 6.841 25.371 1.00 30.71
     ATOM 1893 CG2 VAL 404
                               -0.338 5.528 28.752 1.00 33.24
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    ATOM 1894 C VAL 404
     ATOM 1895 O VAL 404
                               -0.386 4.305 28.914 1.00 30.71
                               0.526 6.309 29.392 1.00 33.66
     ATOM 1896 N PHE 405
     ATOM 1897 CA PHE 405
                                1.516 5.752 30.308 1.00 33.66
     ATOM 1898 CB PHE 405
                                2.901 6.326 29.984 1.00 34.35
     ATOM 1899 CG PHE 405
                                3.343 6.076 28.568 1.00 34.35
45
                                 3.519 7.134 27.683 1.00 34.35
     ATOM 1900 CD1 PHE 405
                                 3.569 4.782 28.114 1.00 34.35
     ATOM 1901 CD2 PHE 405
                                3.911 6.906 26.365 1.00 34.35
     ATOM 1902 CE1 PHE 405
                                3.960 4.545 26.798 1.00 34.35
     ATOM 1903 CE2 PHE 405
                                4.131 5.610 25.922 1.00 34.35
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    ATOM 1904 CZ PHE 405
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ATOM 1905 C PHE 405
                               1.189 5.931 31.790 1.00 33.66
     ATOM 1906 O PHE 405
                               2.036 5.539 32.623 1.00 34.35
     ATOM 1907 OXT PHE 405
                                 0.090 6.434 32.107 1.00 34.35
     ATOM 1908 C1 TRI
                              8.375 7.063 18.475 1.00 34.21
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    ATOM 1909 C2 TRI
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     ATOM 1910 C3 TRI
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    ATOM 1911 C4 TRI
    ATOM 1912 C5 TRI
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    ATOM 1913 C6 TRI
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    ATOM 1914 C7 TRI
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    ATOM 1915 C8 TRI
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    ATOM 1916 C9 TRI
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    ATOM 1917 C10 TRI
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     ATOM 1918 C11 TRI
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                              9.125 7.756 23.490 1.00 33.36
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    ATOM 1921 C15 TRI
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     ATOM 1923 I2 TRI
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                          1
     ATOM 1929 O1 HOH 501
                                9.189 2.098 11.091 1.00 33.36
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     ATOM 1930 O1 HOH 503
                                5.152 5.261 12.137 1.00 33.36
                                3.970 5.057 16.390 1.00 33.36
     ATOM 1931 O1 HOH 504
    ATOM 1932 O1 HOH 534
                                8.296 -0.941 8.998 1.00 33.36
     ATOM 1933 O1 HOH 538
                                4.845 14.369 13.635 1.00 33.36
     ATOM 1934 O1 HOH 540
                                5.789 12.049 10.352 1.00 33.36
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                                5.721 2.525 28.939 1.00 33.36
     ATOM 1936 O1 HOH 555
    ATOM 1937 O1 HOH 556
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    ATOM 1935 O1 HOH 600
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     ATOM 1938 AS1 CAD 701
                                1.863 1.579 0.837 1.00 37.00
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     ATOM 1939 C2 CAD 701
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     ATOM 1940 C3 CAD 701
                                3.511 1.872 1.858 1.00 28.02
                                1.785 2.506 -0.433 1.00 28.02
    ATOM 1941 O4 CAD 701
     ATOM 1942 O5 CAD 701
                                0.592 2.019 1.654 1.00 28.02
     ATOM 1943 AS AS 801
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                                                              AS
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     ATOM 1944 AS AS
                         802
                                                             AS
40
     ATOM 1945 AS AS 803
                              -14.931 -11.763 25.324 1.00 37.00
    END
```

APPENDIX 5

TR_IPBR2.PDB

REMARK rTR_ipbr2 full length numbering

REMARK

5 REMARK Rfactor 0.214 Rfree 0.224

REMARK Resolution 15. 2.2 all reflections

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392

10 REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor

density;

REMARK however, residue name reflects true residue for clarity

15 REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

20 REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY, N.D.ZILZ,

25 N.L.MCCREARY, M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES FOR

TWO

30 JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC V. 263 25 1988

JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS
JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE

JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMON RECEPTOR

35 EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE V. 237 1987

JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED

40 BY

ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR

GENE

TRANSCRIPT

45 JRNL REF NUC. ACIDS. RES. V. 16 12 1988

REMARK

ATOM 1 CB ARG 157 68.481 10.663 6.906 1.00 57.50

ATOM 2 CG ARG 157 69.793 10.213 7.512 1.00 59.93

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3 CD ARG 157
                               70.510 11.365 8.189 1.00 70.24
    ATOM
             4 NE ARG 157
                               71.661 10.906 8.961 1.00 77.62
    ATOM
                               71.599 10.492 10.224 1.00 78.75
             5 CZ ARG 157
    ATOM
                               70.440 10.480 10.870 1.00 74.33
             6 NH1 ARG 157
    ATOM
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    ATOM
             7 NH2 ARG 157
                              66,314 10.014 5.809 1.00 46.84
             8 C ARG 157
    ATOM
                              66.109 10.397 4.659 1.00 54.49
    ATOM
             9 O ARG 157
                              68.442 9.069 5.013 1.00 56.54
             10 N ARG 157
    ATOM
                               67.704 9.537 6.222 1.00 52.92
             11 CA ARG 157
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             12 N PRO 158
    ATOM
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                               65.503 9.448 8.099 1.00 41.72
             13 CD PRO 158
    ATOM
                               63.946 10.368 6.487 1.00 34.98
             14 CA PRO 158
    ATOM
                               63.282 10.172 7.854 1.00 34.92
             15 CB PRO 158
    ATOM
                               64.096 9.096 8.487 1.00 45.83
             16 CG PRO 158
    ATOM
                              63.765 11.804 5.992 1.00 34.13
             17 C PRO 158
15
     ATOM
                              64.223 12.757 6.621 1.00 31.07
             18 O PRO 158
     ATOM
                               63.110 11.932 4.841 1.00 31.36
             19 N GLU 159
    ATOM
                               62.814 13.220 4.228 1.00 27.34
             20 CA GLU 159
    ATOM
                               62.569 13.041 2.726 1.00 24.27
             21 CB GLU 159
     ATOM
                               63.814 12.866 1.887 1.00 24.85
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     ATOM
             22 CG GLU 159
                               64.409 14.188 1.454 1.00 28.12
     ATOM
             23 CD GLU 159
             24 OE1 GLU 159
                                63.642 15.144 1.224 1.00 29.26
     ATOM
                                65.646 14.269 1.326 1.00 29.52
             25 OE2 GLU 159
     ATOM
                               61.528 13.707 4.870 1.00 24.30
     ATOM
             26 C GLU 159
                               60.855 12.934 5.566 1.00 29.01
     ATOM
             27 O GLU 159
25
                              61.192 14.989 4.718 1.00 24.62
             28 N PRO 160
     ATOM
                               61.979 16.126 4.188 1.00 18.72
     ATOM
             29 CD PRO 160
     ATOM
             30 CA PRO 160
                               59.947 15.451 5.330 1.00 21.62
             31 CB PRO 160
                               59.945 16.955 5.048 1.00 12.71
     ATOM
                               61.394 17.297 4.930 1.00 15.12
30
     ATOM
             32 CG PRO 160
     ATOM
             33 C PRO 160
                              58.743 14.752 4.671 1.00 24.61
             34 O PRO 160
                               58.789 14.384 3.490 1.00 22.63
     ATOM
                               57.705 14.504 5.450 1.00 25.86
             35 N THR 161
     ATOM
             36 CA THR 161
                               56.515 13.864 4.921 1.00 23.77
     ATOM
             37 CB THR 161
                               55.689 13.201 6.048 1.00 21.75
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     ATOM
                                55.178 14.210 6.926 1.00 20.78
             38 OG1 THR 161
     ATOM
                                56.549 12.227 6.847 1.00 18.44
             39 CG2 THR 161
     ATOM
             40 C THR 161
                               55.680 14.967 4.269 1.00 28.67
     ATOM
                               55.917 16.151 4.510 1.00 29.90
             41 O THR 161
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                               54.685 14.597 3.448 1.00 27.79
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     ATOM
             42 N PRO 162
             43 CD PRO 162
                               54.313 13.237 3.019 1.00 23.25
     ATOM
             44 CA PRO 162
                               53.843 15.603 2.795 1.00 26.19
     ATOM
                               52.699 14.766 2.227 1.00 19.89
     ATOM
             45 CB PRO 162
                               53.394 13.492 1.848 1.00 20.63
             46 CG PRO 162
     ATOM
                               53.334 16.661 3.775 1.00 24.81
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     ATOM
             47 C PRO 162
                               53.477 17.863 3.526 1.00 21.10
     ATOM
             48 O PRO 162
                               52.812 16.198 4.911 1.00 26.34
             49 N GLU 163
     ATOM
                                52.266 17.065 5.959 1.00 30.38
             50 CA GLU 163
     ATOM
                                51.640 16.231 7.086 1.00 29.46
             51 CB GLU 163
     ATOM
                                50.482 15.321 6.666 1.00 48.37
50
             52 CG GLU 163
     ATOM
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53 CD GLU 163
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     ATOM
             54 OE1 GLU 163
                                51.890 13.441 6.194 1.00 52.22
     ATOM
             55 OE2 GLU 163
                                50.282 13.886 4.766 1.00 59.14
     ATOM
                               53.353 17.949 6.552 1.00 26.74
     ATOM
             56 C GLU 163
             57 O GLU 163
                               53.109 19.107 6.898 1.00 27.03
     ATOM
                               54.553 17.389 6.677 1.00 26.74
             58 N GLU 164
    ATOM
                                55.679 18.124 7.221 1.00 23.65
             59 CA GLU 164
     ATOM
             60 CB GLU 164
                                56.805 17.174 7.609 1.00 18.85
     ATOM
             61 CG GLU 164
                                56.441 16.306 8.804 1.00 26.81
    ATOM
                                57.536 15.334 9.188 1.00 31.06
             62 CD GLU 164
     ATOM
10
             63 OE1 GLU 164
                                58.404 15.050 8.340 1.00 29.21
    ATOM
                                57.524 14.848 10.340 1.00 31.39
             64 OE2 GLU 164
    ATOM
                               56.165 19.204 6.276 1.00 26.54
             65 C GLU 164
     ATOM
     ATOM
             66 O GLU 164
                               56.609 20.258 6.724 1.00 32.48
                               56.075 18.957 4.971 1.00 23.41
             67 N TRP 165
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    ATOM
                               56.488 19.962 3.998 1.00 20.81
             68 CA TRP 165
     ATOM
                               56.462 19.405 2.573 1.00 18.15
             69 CB TRP 165
     ATOM
                               57.762 18.747 2.164 1.00 15.80
             70 CG TRP 165
     ATOM
                                59.058 19.377 2.064 1.00 15.35
             71 CD2 TRP 165
     ATOM
                                59.959 18.392 1.628 1.00 12.14
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     ATOM
             72 CE2 TRP 165
                                59.527 20.676 2.287 1.00 17.56
     ATOM
             73 CE3 TRP 165
                                57.939 17.449 1.804 1.00 12.78
     ATOM
             74 CD1 TRP 165
                                59.253 17.230 1.484 1.00 16.10
     ATOM
             75 NE1 TRP 165
                                61.318 18.657 1.419 1.00 16.26
     ATOM
             76 CZ2 TRP 165
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     ATOM
             77 CZ3 TRP 165
                                61.760 19.933 1.642 1.00 16.48
     ATOM
             78 CH2 TRP 165
                               55.547 21.151 4.109 1.00 19.66
     ATOM
             79 C TRP 165
     ATOM
             80 O TRP 165
                               55.975 22.295 3.960 1.00 23.61
                               54.269 20.882 4.376 1.00 22.66
             81 N ASP 166
     ATOM
                                53.269 21.943 4.537 1.00 23.35
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     ATOM
             82 CA ASP 166
                                51.863 21.359 4.716 1.00 22.61
     ATOM
             83 CB ASP 166
     ATOM
             84 CG ASP 166
                                51.347 20.681 3.458 1.00 31.41
                                51.816 21.028 2.360 1.00 26.38
             85 OD1 ASP 166
     ATOM
             86 OD2 ASP 166
                                50.464 19.803 3.570 1.00 32.25
     ATOM
                               53.631 22.760 5.773 1.00 26.47
             87 C ASP 166
35
     ATOM
             88 O ASP 166
                               53.694 23.991 5.718 1.00 30.25
     ATOM
             89 N LEU 167
                               53.887 22.054 6.872 1.00 24.12
     ATOM
             90 CA LEU 167
                                54.268 22.663 8.139 1.00 26.44
     ATOM
                                54.596 21.557 9.148 1.00 32.57
             91 CB LEU 167
     ATOM
                                54.659 21.919 10.629 1.00 36.97
             92 CG LEU 167
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     ATOM
             93 CD1 LEU 167
                                53.289 22.402 11.080 1.00 43.83
     ATOM
             94 CD2 LEU 167
                                55.096 20.712 11.448 1.00 34.75
     ATOM
                               55.501 23.533 7.904 1.00 23.19
             95 C LEU 167
     ATOM
                               55.570 24.670 8.368 1.00 28.18
             96 O LEU 167
     ATOM
             97 N ILE 168
                              56.450 22.988 7.147 1.00 19.25
45
     ATOM
                               57.703 23.651 6.801 1.00 17.71
             98 CA ILE 168
     ATOM
                               58.632 22.693 6.006 1.00 14.43
             99 CB ILE 168
     ATOM
             100 CG2 ILE 168
                                59.740 23.451 5.304 1.00 16.71
     ATOM
                                59.219 21.644 6.948 1.00 21.24
             101 CG1 ILE 168
     ATOM
                                60.063 20.588 6.264 1.00 18.18
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     ATOM
             102 CD1 ILE 168
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	ATOM		7.475 24.931 6.002 1.00 28.73
	ATOM		88.064 25.977 6.307 1.00 29.36
	ATOM		56.601 24.866 5.005 1.00 24.43
	ATOM	106 CA HIS 169	56.319 26.027 4.169 1.00 23.64
5	ATOM		55.459 25.631 2.971 1.00 23.55
	ATOM	108 CG HIS 169	56.140 24.683 2.034 1.00 23.82
	ATOM	109 CD2 HIS 169	57.455 24.429 1.824 1.00 19.23
	ATOM	110 ND1 HIS 169	55.450 23.833 1.199 1.00 22.92
	ATOM	111 CE1 HIS 169	56.302 23.089 0.522 1.00 19.56
10	ATOM	112 NE2 HIS 169	57.527 23.431 0.883 1.00 26.00
	ATOM		55.653 27.135 4.962 1.00 19.37
	ATOM		56.069 28.288 4.880 1.00 25.64
	ATOM	115 N VAL 170	54.638 26.782 5.745 1.00 19.88
	ATOM	116 CA VAL 170	53.925 27.758 6.555 1.00 20.28
15	ATOM	117 CB VAL 170	52.755 27.100 7.330 1.00 26.06
	ATOM	118 CG1 VAL 170	52.093 28.109 8.259 1.00 20.15
	ATOM	119 CG2 VAL 170	51.725 26.541 6.352 1.00 18.69
	ATOM	120 C VAL 170	54.886 28.442 7.532 1.00 23.11
	ATOM	121 O VAL 170	54.907 29.672 7.625 1.00 28.86
20	ATOM	122 N ALA 171	55.716 27.644 8.203 1.00 20.48
	ATOM	123 CA ALA 171	56.686 28.146 9.173 1.00 19.84
	ATOM	124 CB ALA 171	57.365 26.985 9.902 1.00 18.07
	ATOM	125 C ALA 171	57.728 29.049 8.512 1.00 20.62
	ATOM	126 O ALA 171	58.033 30.127 9.037 1.00 24.67
25	ATOM	127 N THR 172	58.251 28.632 7.359 1.00 20.65
	ATOM	128 CA THR 172	59.247 29.428 6.640 1.00 18.91
	ATOM	129 CB THR 172	59.755 28.709 5.380 1.00 20.06
	ATOM	130 OG1 THR 172	60.267 27.417 5.734 1.00 20.30
	ATOM	131 CG2 THR 172	60.877 29.516 4.726 1.00 18.38
30	ATOM	132 C THR 172	58.675 30.786 6.235 1.00 24.43
	ATOM	133 O THR 172	59.346 31.815 6.360 1.00 23.54
	ATOM	134 N GLU 173	57.430 30.792 5.766 1.00 24.33
	ATOM	135 CA GLU 173	56.783 32.031 5.361 1.00 25.98
	ATOM	136 CB GLU 173	55.460 31.734 4.651 1.00 28.39
35	ATOM	137 CG GLU 173	54.679 32.974 4.207 1.00 40.39
	ATOM	138 CD GLU 173	55.487 33.951 3.347 1.00 48.33
	ATOM	139 OE1 GLU 173	55.261 35.172 3.478 1.00 51.86
	ATOM	140 OE2 GLU 173	56.334 33.513 2.533 1.00 46.92
	ATOM	141 C GLU 173	56.564 32.953 6.562 1.00 25.57
40	ATOM	142 O GLU 173	56.877 34.141 6.498 1.00 27.76
	ATOM	143 N ALA 174	56.071 32.383 7.664 1.00 25.31
	ATOM	144 CA ALA 174	55.823 33.128 8.900 1.00 22.66
	ATOM	145 CB ALA 174	55.340 32.183 10.000 1.00 18.21
	ATOM	146 C ALA 174	57.097 33.847 9.338 1.00 23.47
45	ATOM	147 O ALA 174	57.056 35.003 9.755 1.00 23.76
	ATOM		58.233 33.168 9.226 1.00 22.22
	ATOM	149 CA HIS 175	59.503 33.769 9.592 1.00 20.21
	ATOM	150 CB HIS 175	60.586 32.700 9.738 1.00 13.82
	ATOM	151 CG HIS 175	61.950 33.261 9.984 1.00 20.53
50	ATOM	152 CD2 HIS 175	62.378 34.221 10.843 1.00 10.04

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	ATOM	153 ND1 HIS 175	63.054 32.890 9.249 1.00 22.39
	ATOM	154 CE1 HIS 175	64.103 33.596 9.640 1.00 13.46
	ATOM	155 NE2 HIS 175	63.715 34.410 10.605 1.00 20.86
	ATOM		59.949 34.822 8.571 1.00 25.39
5	ATOM		60.370 35.920 8.949 1.00 26.31
	ATOM	158 N ARG 176	59.868 34.494 7.284 1.00 23.17
	ATOM	159 CA ARG 176	60.292 35.423 6.239 1.00 24.26
	ATOM	160 CB ARG 176	60.168 34.767 4.872 1.00 30.31
	ATOM	161 CG ARG 176	61.286 33.793 4.576 1.00 39.36
10	ATOM	162 CD ARG 176	61.049 33.139 3.243 1.00 49.23
	ATOM	163 NE ARG 176	62.188 32.346 2.808 1.00 60.62
	ATOM	164 CZ ARG 176	62.230 31.688 1.653 1.00 67.96
	ATOM	165 NH1 ARG 176	61.192 31.731 0.823 1.00 68.84
	ATOM	166 NH2 ARG 176	63.313 30.999 1.321 1.00 67.97
15	ATOM	167 C ARG 176	59.548 36.749 6.267 1.00 23.09
	ATOM	168 O ARG 176	60.163 37.807 6.173 1.00 30.71
	ATOM	169 N SER 177	58.240 36.686 6.488 1.00 22.69
	ATOM	170 CA SER 177	57.416 37.885 6.536 1.00 26.50
	ATOM	171 CB SER 177	55.946 37.520 6.341 1.00 19.42
20	ATOM	172 OG SER 177	55.507 36.611 7.331 1.00 27.68
	ATOM	173 C SER 177	57.574 38.695 7.821 1.00 28.70
	ATOM	174 O SER 177	56.986 39.772 7.948 1.00 34.31
	ATOM	175 N THR 178	58.327 38.165 8.786 1.00 27.42
	ATOM	176 CA THR 178	58.540 38.850 10.060 1.00 21.88
25	ATOM	177 CB THR 178	57.842 38.107 11.228 1.00 23.73
	ATOM	178 OG1 THR 178	58.354 36.776 11.337 1.00 24.26
	ATOM	179 CG2 THR 178	56.344 38.037 10.994 1.00 16.77
	ATOM	180 C THR 178	60.027 39.018 10.375 1.00 23.86
	ATOM	181 O THR 178	60.399 39.439 11.474 1.00 24.64
30	ATOM	182 N ASN 179	60.873 38.690 9.402 1.00 23.79
	ATOM	183 CA ASN 179	62.315 38.813 9.563 1.00 26.01
	ATOM	184 CB ASN 179	63.018 37.607 8.947 1.00 23.77
	ATOM	185 CG ASN 179	64.451 37.495 9.386 1.00 30.79
	ATOM	186 OD1 ASN 179	64.737 37.376 10.575 1.00 36.19
35	ATOM	187 ND2 ASN 179	65.364 37.516 8.432 1.00 35.34
	ATOM	188 C ASN 179	62.767 40.101 8.875 1.00 32.11
	ATOM	189 O ASN 179	62.947 40.136 7.652 1.00 36.36
	ATOM	190 N ALA 180	62.945 41.153 9.670 1.00 34.40
	ATOM	191 CA ALA 180	63.333 42.473 9.179 1.00 28.75
40	ATOM	192 CB ALA 180	63.653 43.390 10.346 1.00 29.96
	ATOM	193 C ALA 180	64.481 42.481 8.182 1.00 37.02
	ATOM	194 O ALA 180	65.518 41.866 8.414 1.00 41.85
	ATOM	195 N GLN 181	64.266 43.163 7.057 1.00 37.15
	ATOM	196 CA GLN 181	65.261 43.306 5.995 1.00 39.33
45	ATOM	197 CB GLN 181	66.572 43.877 6.552 1.00 37.42
	ATOM	198 CG GLN 181	66.420 45.190 7.309 1.00 44.86
	ATOM	199 CD GLN 181	65.779 46.285 6.479 1.00 53.60
	ATOM	200 OE1 GLN 181	64.712 46.793 6.821 1.00 58.51
	ATOM	201 NE2 GLN 181	66.422 46.650 5.378 1.00 63.36
50	ATOM	202 C GLN 181	65.549 42.053 5.164 1.00 44.18

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66.367 42.102 4.239 1.00 46.35
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            203 O GLN 181
            204 N GLY 182
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    ATOM
            205 CA GLY 182
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    ATOM
                               66.531 39.363 4.477 1.00 49.98
            206 C GLY 182
    ATOM
                               67.309 39.175 5.419 1.00 56.26
            207 O GLY 182
    ATOM
                               66.907 39.274 3.205 1.00 50.96
            208 N SER 183
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                               68.281 38.947 2.830 1.00 55.69
    ATOM
            209 CA SER 183
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            210 CB SER 183
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            211 OG SER 183
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    ATOM
            212 C SER 183
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                              70.352 40.138 2.540 1.00 66.02
    ATOM
            213 O SER 183
                              68.453 41.338 2.413 1.00 60.68
            214 N HIS 184
    ATOM
            215 CA HIS 184
                               69.131 42.600 2.139 1.00 60.01
    ATOM
    ATOM
            216 CB HIS 184
                               68.150 43.596 1.517 1.00 53.49
            217 C HIS 184
                              69.798 43.209 3.380 1.00 59.43
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    ATOM
                              70.373 44.300 3.303 1.00 59.56
            218 O HIS 184
     ATOM
            219 N TRP 185
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    ATOM
            220 CA TRP 185
                               70.343 42.995 5.754 1.00 54.25
    ATOM
                               70.147 41.988 6.899 1.00 47.54
    ATOM
            221 CB TRP 185
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    ATOM
            222 CG TRP 185
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                                72.233 40.404 7.230 1.00 39.59
     ATOM
            223 CD2 TRP 185
            224 CE2 TRP 185
                                72.522 39.070 6.874 1.00 30.27
     ATOM
                                73.202 41.146 7.919 1.00 35.23
     ATOM
            225 CE3 TRP 185
    ATOM
            226 CD1 TRP 185
                                70.462 39.553 6.149 1.00 39.73
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    ATOM
            227 NE1 TRP 185
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            228 CZ2 TRP 185
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            229 CZ3 TRP 185
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    ATOM
            230 CH2 TRP 185
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            231 C TRP 185
                               71.818 43.382 5.655 1.00 54.21
     ATOM
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     ATOM
            232 O TRP 185
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     ATOM
            233 N LYS 186
                               72.605 42.584 4.938 1.00 54.57
    ATOM
            234 CA LYS 186
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            235 CB LYS 186
                               74.712 41.682 4.080 1.00 53.31
     ATOM
            236 C LYS 186
                               74.338 44.160 4.061 1.00 58.96
     ATOM
            237 O LYS 186
                               75.417 44.731 4.226 1.00 62.57
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     ATOM
            238 N GLN 187
                               73.382 44.640 3.268 1.00 60.12
     ATOM
                                73.563 45.873 2.512 1.00 60.15
    ATOM
            239 CA GLN 187
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    ATOM
            240 CB GLN 187
                               72.809 47.064 3.101 1.00 60.91
            241 C GLN 187
    ATOM
                               73.149 48.213 2.822 1.00 66.50
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    ATOM
            242 O GLN 187
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     ATOM
            243 N ARG 188
                                70.983 47.847 4.525 1.00 59.26
            244 CA ARG 188
     ATOM
                                69.504 47.462 4.466 1.00 55.21
     ATOM
            245 CB ARG 188
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     ATOM
            246 C ARG 188
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     ATOM
            247 O ARG 188
                               72.202 47.432 6.607 1.00 55.46
     ATOM
            248 N ARG 189
            249 CA ARG 189
                                72.630 47.704 7.979 1.00 52.98
     ATOM
                                73.211 46.437 8.619 1.00 47.73
            250 CB ARG 189
     ATOM
                                74.509 45.985 7.989 1.00 47.88
                         189
     ATOM
            251 CG ARG
                                75.080 44.763 8.654 1.00 46.96
50
            252 CD ARG 189
     ATOM
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ATOM 254 CZ ARG 189 ATOM 255 NH1 ARG 189 ATOM 256 NH2 ARG 189 ATOM 256 NH2 ARG 189 ATOM 257 C ARG 189 ATOM 257 C ARG 189 ATOM 258 O ARG 189 ATOM 259 N LYS 190 ATOM 260 CA LYS 190 ATOM 261 CB LYS 190 ATOM 262 C LYS 190 ATOM 263 O LYS 190 ATOM 264 N PHE 191 ATOM 265 CA PHE 191 ATOM 266 CB PHE 191 ATOM 267 CG PHE 191 ATOM 268 CD1 PHE 191 ATOM 268 CD2 PHE 191 ATOM 270 CEI PHE 191 ATOM 271 CE2 PHE 191 ATOM 273 C PHE 191 ATOM 274 O PHE 191 ATOM 275 N LEU 192 ATOM 276 CA LEU 192 ATOM 276 CA LEU 192 ATOM 277 CB LEU 192 ATOM 278 CG LEU 192 ATOM 280 CD2 LEU 192 ATOM 281 C LEU 192 ATOM 281 C LEU 192 ATOM 282 O LEU 192 ATOM 283 N PRO 193 ATOM 284 CD PRO 193 ATOM 285 CA PRO 193 ATOM 286 CB PRO 193 ATOM 286 CB PRO 193 ATOM 287 CG PRO 193 ATOM 288 C APRO 193 ATOM 288 C APRO 193 ATOM 289 O PRO 193 ATOM 290 CA ASP 194 ATOM 292 CB ASP 194 ATOM 292 CB ASP 194 ATOM 299 CA ASP 195 ATOM 300 CB ASP 195 ATOM 301 CG ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG ASP 194 ATOM 302 OD1 ASP 195 ATOM 302 OD1 ASP 195 ATOM 301 CG ASP 194 ATOM 301 CG ASP 194 ATOM 302 OD1 ASP 195 ATOM 302 OD1 ASP 195 ATOM 302 OD1 ASP 195 ATOM 300 CD1 ASP 194 ATOM 300 CD1 ASP 195 ATOM 300 CD1 ASP 194 ATOM 300 CD1 ASP 194 ATOM 300 CD1 ASP 195		ATOM	253 NE ARG 189	76.377 44.441 8.068 1.00 57.93
ATOM 255 NH1 ARG 189 ATOM 256 NH2 ARG 189 ATOM 257 C ARG 189 ATOM 258 O ARG 189 ATOM 259 N LYS 190 ATOM 260 CA LYS 190 ATOM 261 CB LYS 190 ATOM 262 C LYS 190 ATOM 263 O LYS 190 ATOM 264 N PHE 191 ATOM 265 CA PHE 191 ATOM 266 CB PHE 191 ATOM 267 CG PHE 191 ATOM 268 CD1 PHE 191 ATOM 269 CD2 PHE 191 ATOM 270 CE1 PHE 191 ATOM 271 CE2 PHE 191 ATOM 273 C PHE 191 ATOM 273 C PHE 191 ATOM 275 N LEU 192 ATOM 276 CA LEU 192 ATOM 277 CB LEU 192 ATOM 277 CB LEU 192 ATOM 280 CD2 LEU 192 ATOM 281 C LEU 192 ATOM 282 O LEU 192 ATOM 283 N PRO 193 ATOM 283 N PRO 193 ATOM 284 CD PRO 193 ATOM 285 CA PRO 193 ATOM 286 CB PRO 193 ATOM 287 CG PASP 194 ATOM 289 O PRO 193 ATOM 289 O PRO 193 ATOM 299 CA ASP 194 ATOM 299 CA ASP 194 ATOM 299 CA ASP 194 ATOM 299 CA ASP 195 ATOM 299 CA ASP 194 ATOM 299 CA ASP 195 ATOM 301 CG A			_	
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ATOM 288 C PRO 193 79.475 54.377 17.137 1.00 49.60 ATOM 289 O PRO 193 79.000 54.033 18.218 1.00 54.05 ATOM 290 N ASP 194 80.783 54.383 16.891 1.00 50.63 ATOM 291 CA ASP 194 81.769 53.951 17.885 1.00 54.57 40 ATOM 292 CB ASP 194 83.164 53.965 17.272 1.00 59.28 ATOM 293 CG ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 300 CB ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67	35			
ATOM 289 O PRO 193 79.000 54.033 18.218 1.00 54.05 ATOM 290 N ASP 194 80.783 54.383 16.891 1.00 50.63 ATOM 291 CA ASP 194 81.769 53.951 17.885 1.00 54.57 40 ATOM 292 CB ASP 194 83.164 53.965 17.272 1.00 59.28 ATOM 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.268 55.956 19.168 1.00 59.68 ATOM 300 CB ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67	33			
ATOM 290 N ASP 194 80.783 54.383 16.891 1.00 50.63 ATOM 291 CA ASP 194 81.769 53.951 17.885 1.00 54.57 40 ATOM 292 CB ASP 194 83.164 53.965 17.272 1.00 59.28 ATOM 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				
ATOM 291 CA ASP 194 81.769 53.951 17.885 1.00 54.57 40 ATOM 292 CB ASP 194 83.164 53.965 17.272 1.00 59.28 ATOM 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				
40 ATOM 292 CB ASP 194 83.164 53.965 17.272 1.00 59.28 ATOM 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67		•		
ATOM 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67	40			
ATOM 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				
ATOM 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				
ATOM 296 C ASP 194 81.769 54.726 19.198 1.00 54.41 45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				83.640 51.787 16.486 1.00 69.00
45 ATOM 297 O ASP 194 82.229 54.221 20.222 1.00 55.27 ATOM 298 N ASP 195 81.268 55.956 19.168 1.00 57.20 ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				81.769 54.726 19.198 1.00 54.41
ATOM 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67	45	ATOM	297 O ASP 194	82.229 54.221 20.222 1.00 55.27
ATOM 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67				81.268 55.956 19.168 1.00 57.20
ATOM 301 CG ASP 195 79.747 58.526 19.187 1.00 71.67		ATOM		81.206 56.775 20.371 1.00 59.68
		ATOM		81.017 58.261 20.006 1.00 62.99
50 ATOM 302 OD1 ASP 195 78.734 58.956 19.796 1.00 70.17				
	50	ATOM	302 OD1 ASP 195	78.734 58.956 19.796 1.00 70.17

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ATOM
            303 OD2 ASP 195
                                79.782 58.311 17.951 1.00 75.23
                              80.092 56.289 21.306 1.00 58.39
    ATOM
            304 C ASP 195
            305 O ASP 195
                              80.032 56.676 22.474 1.00 59.81
    ATOM
                              79.245 55.399 20.794 1.00 54.47
            306 N ILE 196
     ATOM
            307 CA ILE 196
                               78.141 54.840 21.568 1.00 49.00
    ATOM
5
                               76.839 54.780 20.731 1.00 46.64
            308 CB ILE 196
    ATOM
            309 CG2 ILE 196
                               75.701 54.195 21.560 1.00 42.11
    ATOM
                               76.467 56.184 20.241 1.00 44.23
           310 CG1 ILE 196
    ATOM
                               75.214 56.238 19.373 1.00 48.45
    ATOM 311 CD1 ILE 196
                              78.497 53.436 22.068 1.00 46.22
            312 C ILE 196
10
    ATOM
                              78.912 52.570 21.298 1.00 42.07
    ATOM
            313 O ILE 196
                               78.357 53.228 23.370 1.00 45.62
           314 N GLY 197
    ATOM
                                78.658 51.930 23.941 1.00 51.49
            315 CA GLY 197
    ATOM
                               80.005 51.832 24.625 1.00 54.64
    ATOM
            316 C GLY 197
            317 O GLY 197
                               80.377 50.759 25.092 1.00 49.98
    ATOM
15
            318 N GLN 198
                               80.726 52.946 24.725 1.00 60.08
    ATOM
    ATOM
            319 CA GLN 198
                                82.039 52.939 25.366 1.00 61.01
            320 CB GLN 198
                                83.082 53.568 24.441 1.00 55.55
     ATOM
            321 C GLN 198
                               82.044 53.633 26.733 1.00 59.57
     ATOM
                               83.103 54.016 27.232 1.00 61.30
            322 O GLN 198
20
     ATOM
            323 N SER 199
                               80.875 53.738 27.362 1.00 57.27
     ATOM
            324 CA SER 199
                               80.758 54.397 28.665 1.00 50.61
     ATOM
            325 CB SER 199
                               80.276 55.842 28.478 1.00 53.70
     ATOM
                               81.010 56.508 27.463 1.00 61.92
     ATOM
            326 OG SER 199
           327 C SER 199
                              79.848 53.684 29.675 1.00 46.41
25
     ATOM
                               78.798 54.210 30.060 1.00 41.16
     ATOM
            328 O SER 199
                               80.222 52.466 30.096 1.00 42.08
     ATOM
            329 N PRO 200
                                81.349 51.648 29.605 1.00 38.31
     ATOM
            330 CD PRO 200
                                79.409 51.722 31.065 1.00 44.04
     ATOM
            331 CA PRO 200
                                79.941 50.297 30.925 1.00 36.06
30
     ATOM
            332 CB PRO 200
                                81.377 50.504 30.583 1.00 37.43
     ATOM
            333 CG PRO 200
     ATOM
            334 C PRO 200
                               79.615 52.270 32.485 1.00 50.91
     ATOM
            335 O PRO 200
                               80.629 51.980 33.123 1.00 55.65
     ATOM
            336 N ILE 201
                              78.663 53.060 32.975 1.00 55.81
     ATOM
            337 CA ILE 201
                               78.781 53.651 34.311 1.00 57.24
35
            338 CB ILE 201
                               78.861 55.192 34.250 1.00 58.40
     ATOM
                               80.218 55.622 33.709 1.00 60.49
            339 CG2 ILE 201
     ATOM
     ATOM
            340 CG1 ILE 201
                               77.716 55.751 33.404 1.00 62.42
            341 CD1 ILE 201
                               77.819 57.234 33.137 1.00 61.68
     ATOM
            342 C ILE 201
                              77.728 53.241 35.332 1.00 56.52
40
     ATOM
     ATOM
            343 O ILE 201
                              77.961 53.352 36.537 1.00 60.89
                               76.564 52.794 34.871 1.00 52.76
            344 N VAL 202
     ATOM
                                75.522 52.366 35.802 1.00 47.37
            345 CA VAL 202
     ATOM
                                74.117 52.377 35.153 1.00 38.14
            346 CB VAL 202
     ATOM
                                73.092 51.804 36.117 1.00 30.35
            347 CG1 VAL 202
45
     ATOM
            348 CG2 VAL 202
                                73,730 53,798 34,763 1.00 26,69
     ATOM
            349 C VAL 202
                               75.885 50.958 36.285 1.00 53.65
     ATOM
            350 O VAL 202
                               75.914 50.010 35.500 1.00 55.10
     ATOM
            351 N SER 203
                               76.226 50.839 37.561 1.00 59.85
     ATOM
           352 CA SER 203
                               76.614 49.556 38.132 1.00 64.58
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     ATOM
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	ATOM	353 CB SER 203	77.209 49.749 39.532 1.00 68.95
	ATOM	354 OG SER 203	78.396 50.523 39.483 1.00 74.02
	ATOM	355 C SER 203	75.493 48.528 38.197 1.00 61.69
	ATOM	356 O SER 203	74.351 48.846 38.535 1.00 63.63
5	ATOM	357 N MET 204	75.848 47.295 37.859 1.00 57.37
	ATOM	358 CA MET 204	74.932 46.162 37.885 1.00 57.54
	ATOM	359 CB MET 204	74.847 45.505 36.501 1.00 56.59
	ATOM	360 CG MET 204	74.012 46.270 35.489 1.00 44.08
	ATOM	361 SD MET 204	72.255 46.228 35.884 1.00 46.62
10	ATOM	362 CE MET 204	71.775 44.758 35.013 1.00 48.37
	ATOM	363 C MET 204	75.522 45.178 38.888 1.00 55.86
	ATOM	364 O MET 204	76.746 45.089 39.027 1.00 58.94
	ATOM	365 N PRO 205	74.671 44.432 39.607 1.00 55.36
	ATOM	366 CD PRO 205	73.203 44.570 39.625 1.00 57.73
15	ATOM	367 CA PRO 205	75.119 43.453 40.604 1.00 56.82
	ATOM	368 CB PRO 205	73.814 43.042 41.295 1.00 59.79
	ATOM	369 CG PRO 205	72.769 43.281 40.255 1.00 57.85
	ATOM	370 C PRO 205	75.902 42.239 40.083 1.00 57.25
	ATOM	371 O PRO 205	75.683 41.118 40.541 1.00 66.28
20	ATOM	372 N ASP 206	76.822 42.462 39.147 1.00 58.75
	ATOM	373 CA ASP 206	77.639 41.389 38.586 1.00 61.09
	ATOM	374 CB ASP 206	76.802 40.462 37.685 1.00 66.07
	ATOM	375 CG ASP 206	76.158 41.190 36.521 1.00 70.97
	ATOM	376 OD1 ASP 206	74.989 41.613 36.662 1.00 76.97
25	ATOM	377 OD2 ASP 206	76.813 41.322 35.465 1.00 61.12
	ATOM	378 C ASP 206	78.865 41.910 37.832 1.00 61.96
	ATOM	379 O ASP 206	79.406 41.230 36.957 1.00 65.14
	ATOM	380 N GLY 207	79.282 43.130 38.158 1.00 63.00
	ATOM	381 CA GLY 207	80.455 43.709 37.522 1.00 64.43
30	ATOM	382 C GLY 207	80.224 44.467 36.229 1.00 64.81
	ATOM	383 O GLY 207	80.649 45.619 36.110 1.00 68.76
	ATOM	384 N ASP 208	79.584 43.827 35.253 1.00 63.53
	ATOM	385 CA ASP 208	79.316 44.459 33.962 1.00 58.96
	ATOM	386 CB ASP 208	78.746 43.434 32.974 1.00 62.84
35	ATOM	387 CG ASP 208	79.743 42.336 32.633 1.00 64.73
	ATOM	388 OD1 ASP 208	79.575 41.200 33.121 1.00 66.65
	ATOM	389 OD2 ASP 208	80.701 42.610 31.878 1.00 68.91
	ATOM	390 C ASP 208	78.368 45.646 34.110 1.00 56.65
	ATOM	391 O ASP 208	77.182 45.473 34.392 1.00 55.79
40	ATOM	392 N LYS 209	78.911 46.852 33.953 1.00 54.66
	ATOM	393 CA LYS 209	78.132 48.081 34.082 1.00 53.92
	ATOM	394 CB LYS 209	79.034 49.236 34.515 1.00 49.71
	ATOM	395 C LYS 209	77.395 48.420 32.785 1.00 48.30
	ATOM	396 O LYS 209	77.767 47.945 31.711 1.00 45.62
45	ATOM	397 N VAL 210	76.367 49.258 32.894 1.00 43.87
	ATOM	398 CA VAL 210	75.539 49.662 31.757 1.00 41.25
	ATOM	399 CB VAL 210	74.020 49.624 32.125 1.00 32.99
	ATOM	400 CG1 VAL 210	73.153 50.029 30.937 1.00 31.44
	ATOM	401 CG2 VAL 210	73.626 48.239 32.604 1.00 27.57
50	ATOM	402 C VAL 210	75.868 51.061 31.234 1.00 43.30

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76.261 51.951 31.994 1.00 44.65
    ATOM
            403 O VAL 210
            404 N ASP 211
                              75.688 51.235 29.931 1.00 43.23
    ATOM
                               75.906 52.498 29.240 1.00 40.62
            405 CA ASP 211
    ATOM
                               76.686 52.232 27.943 1.00 43.49
            406 CB ASP 211
    ATOM
                               77.014 53.499 27.161 1.00 40.77
            407 CG ASP 211
    ATOM
                                76.180 54.427 27.092 1.00 42.13
            408 OD1 ASP 211
    ATOM
                                78.111 53.549 26.574 1.00 37.49
            409 OD2 ASP 211
    ATOM
                               74.491 53.001 28.921 1.00 44.56
            410 C ASP 211
    ATOM
                               73.849 52.500 27.998 1.00 46.44
            411 O ASP 211
    ATOM
                               74.006 53,982 29.684 1.00 43.76
            412 N LEU 212
10
    ATOM
                                72.662 54.538 29.494 1.00 41.47
            413 CA LEU 212
    ATOM
                                72.473 55.785 30.359 1.00 40.45
            414 CB LEU 212
    ATOM
                                72.360 55.585 31.867 1.00 44.47
            415 CG LEU 212
    ATOM
                                72.127 56.923 32.551 1.00 40.49
            416 CD1 LEU 212
    ATOM
                                71.217 54.634 32.153 1.00 45.94
            417 CD2 LEU 212
15
    ATOM
                               72.325 54.886 28.049 1.00 40.77
            418 C LEU 212
    ATOM
                               71,254 54,540 27,548 1.00 42.25
            419 O LEU 212
    ATOM
                               73.241 55.588 27.394 1.00 42.53
            420 N GLU 213
    ATOM
                                73.068 56.008 26.009 1.00 43.60
    ATOM
            421 CA GLU 213
                                74.267 56.860 25.598 1.00 43.84
20
    ATOM
            422 CB GLU 213
                                74.246 57.334 24.167 1.00 51.70
    ATOM
            423 CG GLU 213
            424 CD GLU 213
                                75.598 57.848 23.722 1.00 59.23
     ATOM
            425 OE1 GLU 213
                                 75.655 58.939 23.121 1.00 60.14
     ATOM
                                76.611 57.158 23.980 1.00 64.78
     ATOM
            426 OE2 GLU 213
                               72.913 54.810 25.066 1.00 42.63
            427 C GLU 213
     ATOM
25
                               72.008 54.779 24.226 1.00 37.04
            428 O GLU 213
     ATOM
                               73.775 53.814 25.245 1.00 39.28
             429 N ALA 214
     ATOM
                                73.753 52.605 24.424 1.00 39.52
             430 CA ALA 214
     ATOM
                                74.952 51.726 24.740 1.00 35.16
             431 CB ALA 214
     ATOM
             432 C ALA 214
                               72.460 51.852 24.694 1.00 37.14
     ATOM
30
                               71.795 51.390 23.767 1.00 42.29
     ATOM
             433 O ALA 214
                               72.098 51.773 25.970 1.00 31.60
             434 N PHE 215
     ATOM
                                70.883 51.102 26.404 1.00 31.67
             435 CA PHE 215
     ATOM
                                70.728 51.217 27.922 1.00 24.80
            436 CB PHE 215
     ATOM
                                69.512 50.522 28.458 1.00 21.78
            437 CG PHE 215
35
     ATOM
                                69.553 49.171 28.771 1.00 24.64
             438 CD1 PHE 215
     ATOM
                                68.328 51.223 28.658 1.00 21.53
             439 CD2 PHE 215
     ATOM
                                68.429 48.528 29.277 1.00 27.63
             440 CE1 PHE 215
     ATOM
                                67.200 50.591 29.163 1.00 21.60
             441 CE2 PHE 215
     ATOM
                                67.249 49.242 29.472 1.00 21.35
             442 CZ PHE 215
     ATOM
40
                               69.675 51.706 25.694 1.00 35.75
             443 C PHE 215
     ATOM
                               68.838 50.975 25.161 1.00 34.84
             444 O PHE 215
     ATOM
                               69.604 53.035 25.665 1.00 39.09
             445 N SER 216
     ATOM
                                68.506 53.739 25.001 1.00 40.61
     ATOM
             446 CA SER 216
                                68.668 55.249 25.165 1.00 43.86
             447 CB SER 216
     ATOM
45
                                68.616 55.603 26.537 1.00 68.66
             448 OG SER 216
     ATOM
                               68.444 53.380 23.518 1.00 40.76
             449 C SER 216
     ATOM
             450 O SER 216
                               67.362 53.161 22.969 1.00 35.50
     ATOM
                                69.611 53.332 22.878 1.00 38.37
             451 N GLU 217
     ATOM
                               69.709 52.989 21.462 1.00 37.80
            452 CA GLU 217
50
     ATOM
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453 CB GLU 217
                                71.164 53.049 20.997 1.00 39.67
    ATOM
                                71.701 54.461 20.880 1.00 46.65
            454 CG GLU 217
    ATOM
            455 CD GLU 217
                                70.881 55.315 19.925 1.00 53.25
    ATOM
                                70.920 55.056 18.702 1.00 57.12
            456 OE1 GLU 217
    ATOM
                                70.189 56.240 20.400 1.00 54.13
            457 OE2 GLU 217
    ATOM
                               69.135 51.598 21.209 1.00 38.48
    ATOM
            458 C GLU 217
    ATOM 459 O GLU 217
                               68.416 51.378 20.228 1.00 43.00
                               69.426 50.677 22.120 1.00 35.49
    ATOM 460 N PHE 218
            461 CA PHE 218
                               68.934 49.313 22.018 1.00 31.76
    ATOM
                               69.743 48.392 22.925 1.00 29.10
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    ATOM
            462 CB PHE 218
            463 CG PHE 218
                               71.169 48.260 22.510 1.00 26.25
    ATOM
    ATOM
            464 CD1 PHE 218
                                72.176 48.177 23.459 1.00 24.59
                                71.510 48.233 21.163 1.00 23.53
    ATOM
            465 CD2 PHE 218
            466 CE1 PHE 218
                                73.504 48.072 23.073 1.00 27.68
     ATOM
                                72.832 48.128 20.765 1.00 25.37
    ATOM
            467 CE2 PHE 218
15
    ATOM
            468 CZ PHE 218
                               73.834 48.047 21.721 1.00 28.43
            469 C PHE 218
                               67.445 49.202 22.321 1.00 31.30
    ATOM
                               66.726 48.496 21.621 1.00 35.18
    ATOM
            470 O PHE 218
            471 N THR 219
                               66.967 49.915 23.333 1.00 30.54
    ATOM
            472 CA THR 219
                                65.552 49.853 23.675 1.00 33.53
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    ATOM
            473 CB THR 219
                                65.269 50.467 25.057 1.00 36.07
     ATOM
            474 OG1 THR 219
                                65.903 51.746 25.157 1.00 42.99
     ATOM
                                65.797 49.562 26.145 1.00 34.32
    ATOM
            475 CG2 THR 219
            476 C THR 219
                               64.680 50.514 22.609 1.00 34.53
     ATOM
                               63.507 50.162 22.450 1.00 36.57
    ATOM
            477 O THR 219
25
                               65.267 51.457 21.873 1.00 38.13
     ATOM
            478 N LYS 220
                               64.563 52.158 20.806 1.00 41.42
     ATOM
            479 CA LYS 220
            480 CB LYS 220
                               65.452 53.257 20.208 1.00 41.62
     ATOM
            481 C LYS 220
                               64.140 51.182 19.716 1.00 41.80
     ATOM
            482 O LYS 220
                               63.032 51.274 19.192 1.00 43.29
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    ATOM
            483 N ILE 221
                              65.018 50.234 19.393 1.00 36.93
     ATOM
                               64.726 49.250 18.355 1.00 37.33
            484 CA ILE 221
     ATOM
            485 CB ILE 221
                               65.965 48.932 17.482 1.00 33.71
     ATOM
     ATOM 486 CG2 ILE 221
                               66.491 50.202 16.826 1.00 41.26
     ATOM 487 CG1 ILE 221
                               67.042 48.235 18.309 1.00 30.36
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     ATOM 488 CD1 ILE 221
                               68.178 47.687 17.472 1.00 26.28
     ATOM 489 C ILE 221
                              64.141 47.922 18.845 1.00 40.49
                              63.593 47.159 18.048 1.00 43.43
            490 O ILE 221
     ATOM
                              64.219 47.651 20.144 1.00 39.43
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            491 N ILE 222
                               63.703 46.394 20.667 1.00 35.49
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     ATOM
            492 CA ILE 222
            493 CB ILE 222
                               64.169 46.133 22.130 1.00 34.06
     ATOM
            494 CG2 ILE 222
                               63.287 46.881 23.130 1.00 26.15
     ATOM
     ATOM
            495 CG1 ILE 222
                               64.155 44.627 22.405 1.00 34.08
            496 CD1 ILE 222
                               64.760 44.220 23.719 1.00 33.67
     ATOM
            497 C ILE 222
                              62.186 46.230 20.539 1.00 37.60
     ATOM
            498 O ILE 222
                              61.703 45.127 20.279 1.00 42.14
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     ATOM 499 N THR 223
                               61.438 47.324 20.665 1.00 34.60
                                59.979 47.257 20.562 1.00 35.96
     ATOM 500 CA THR 223
            501 CB THR 223
                                59.323 48.645 20.799 1.00 41.70
     ATOM
            502 OG1 THR 223
                                59.681 49.119 22.106 1.00 44.59
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     ATOM
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57.796 48.548 20.706 1.00 42.58
            503 CG2 THR 223
    ATOM
            504 C THR 223
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    ATOM
                              58.671 45.680 19.289 1.00 30.60
            505 O THR 223
    ATOM
            506 N PRO 224
                              59,942 47,103 18,084 1,00 31,99
    ATOM
           507 CD PRO 224
                               60.784 48.288 17.839 1.00 30.37
    ATOM
5
                               59.496 46.517 16.815 1.00 29.25
            508 CA PRO 224
    ATOM
                               60.225 47.366 15.769 1.00 29.27
           509 CB PRO 224
    ATOM
                               60.393 48.677 16.441 1.00 36.31
    ATOM 510 CG PRO 224
                              59.913 45.050 16.723 1.00 29.20
    ATOM 511 C PRO 224
                              59.146 44.209 16.251 1.00 33.73
    ATOM 512 O PRO 224
10
                              61.124 44.754 17.192 1.00 19.86
    ATOM 513 N ALA 225
                               61.663 43.395 17.175 1.00 19.61
           514 CA ALA 225
    ATOM
                               63.086 43.388 17.730 1.00 19.08
            515 CB ALA 225
    ATOM
            516 C ALA 225
                              60.777 42.428 17.960 1.00 20.48
    ATOM
                              60.474 41.331 17.489 1.00 24.33
            517 O ALA 225
15
    ATOM
                              60,330 42.847 19.141 1.00 23.72
            518 N ILE 226
    ATOM
           519 CA ILE 226
                              59.471 42.001 19.972 1.00 21.94
    ATOM
                              59.152 42.667 21.333 1.00 21.01
    ATOM 520 CB ILE 226
                               58.118 41.846 22.095 1.00 15.14
    ATOM 521 CG2 ILE 226
                               60.425 42.841 22.163 1.00 20.45
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    ATOM 522 CG1 ILE 226
                               60.216 43.741 23.358 1.00 17.65
    ATOM 523 CD1 ILE 226
                              58.165 41.758 19.228 1.00 24.04
     ATOM 524 C ILE 226
                              57.640 40.642 19.220 1.00 26.92
     ATOM
           525 O ILE 226
                              57.653 42.811 18.596 1.00 25.22
     ATOM 526 N THR 227
                               56.410 42.730 17.836 1.00 27.92
     ATOM 527 CA THR 227
25
                               55,984 44.132 17.333 1.00 34.33
           528 CB THR 227
     ATOM
                                55.823 45.007 18.458 1.00 33.62
     ATOM 529 OG1 THR 227
                                54.669 44.061 16.563 1.00 39.18
     ATOM 530 CG2 THR 227
                              56.524 41.733 16.671 1.00 23.61
     ATOM 531 C THR 227
                               55,587 40,977 16,413 1.00 24,41
     ATOM
            532 O THR 227
30
                               57.670 41.704 15.995 1.00 15.49
     ATOM 533 N ARG 228
     ATOM 534 CA ARG 228
                               57.872 40.773 14.885 1.00 17.92
     ATOM 535 CB ARG 228
                               59.174 41.075 14.137 1.00 19.84
                               59.203 42.437 13.452 1.00 20.62
           536 CG ARG 228
     ATOM
           537 CD ARG 228
                               60.351 42.523 12.453 1.00 24.29
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     ATOM
            538 NE ARG 228
                               61.641 42.168 13.047 1.00 27.04
     ATOM
                               62.452 43.039 13.642 1.00 37.92
            539 CZ ARG 228
     ATOM
                                62.113 44.327 13.725 1.00 42.82
            540 NH1 ARG 228
     ATOM
                                63.618 42.634 14.136 1.00 34.80
     ATOM 541 NH2 ARG 228
                               57.870 39.323 15.387 1.00 22.51
     ATOM 542 C ARG 228
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                               57.402 38.421 14.686 1.00 28.49
     ATOM 543 O ARG 228
                               58.362 39.104 16.607 1.00 21.46
     ATOM 544 N VAL 229
            545 CA VAL 229
                                58.372 37.762 17.187 1.00 20.12
     ATOM
     ATOM 546 CB VAL 229
                               59.149 37.707 18.524 1.00 17.21
                                59.023 36.322 19.152 1.00 13.73
45
     ATOM 547 CG1 VAL 229
                                60.611 38.019 18.287 1.00 15.80
     ATOM 548 CG2 VAL 229
     ATOM 549 C VAL 229
                               56.926 37.348 17.421 1.00 19.19
                               56.528 36.224 17.089 1.00 19.86
     ATOM 550 O VAL 229
                               56.134 38.275 17.953 1.00 21.49
            551 N VAL 230
     ATOM
                               54.721 38.023 18.217 1.00 17.69
     ATOM 552 CA VAL 230
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	ATOM	553 CB VAL 230	54.041 39.239 18.881 1.00 21.30
	ATOM	554 CG1 VAL 230	52.568 38.952 19.090 1.00 17.26
	ATOM	555 CG2 VAL 230	54.706 39.572 20.218 1.00 17.13
	ATOM	556 C VAL 230	54.003 37.707 16.902 1.00 26.39
5	ATOM	557 O VAL 230	53.180 36.790 16.843 1.00 29.63
	ATOM	558 N ASP 231	54.333 38.451 15.848 1.00 25.52
	ATOM	559 CA ASP 231	53.724 38.242 14.537 1.00 26.78
	ATOM	560 CB ASP 231	54.132 39.353 13.571 1.00 23.70
	ATOM	561 CG ASP 231	53.649 40.728 14.012 1.00 31.60
10	ATOM	562 OD1 ASP 231	52.656 40.820 14.771 1.00 31.79
	ATOM	563 OD2 ASP 231	54.271 41.727 13.593 1.00 35.74
	ATOM	564 C ASP 231	54.108 36.879 13.970 1.00 27.69
	ATOM	565 O ASP 231	53.279 36.196 13.366 1.00 25.15
	ATOM	566 N PHE 232	55.364 36.490 14.170 1.00 22.29
15	ATOM	567 CA PHE 232	55.858 35.200 13.703 1.00 23.78
	ATOM	568 CB PHE 232	57.328 35.008 14.097 1.00 24.76
	ATOM	569 CG PHE 232	57.794 33.581 14.017 1.00 25.63
	ATOM	570 CD1 PHE 232	58.000 32.967 12.785 1.00 24.50
	ATOM	571 CD2 PHE 232	57.980 32.830 15.181 1.00 19.35
20	ATOM	572 CE1 PHE 232	58.381 31.630 12.705 1.00 22.27
	ATOM	573 CE2 PHE 232	58.359 31.496 15.114 1.00 20.63
	ATOM	574 CZ PHE 232	58.561 30.893 13.873 1.00 26.10
	ATOM	575 C PHE 232	55.018 34.093 14.328 1.00 23.51
	ATOM	576 O PHE 232	54.541 33.189 13.637 1.00 22.39
25	ATOM	577 N ALA 233	54.837 34.182 15.644 1.00 24.55
	ATOM	578 CA ALA 233	54.070 33.192 16.387 1.00 23.10
	ATOM	579 CB ALA 233	54.145 33.490 17.869 1.00 17.99
	ATOM	580 C ALA 233	52.616 33.137 15.929 1.00 27.99
•	ATOM	581 O ALA 233	52.063 32.051 15.744 1.00 25.71
30	ATOM	582 N LYS 234	51.997 34.305 15.760 1.00 30.19
	ATOM	583 CA LYS 234	50.601 34.380 15.325 1.00 31.58
	ATOM	584 CB LYS 234 585 CG LYS 234	50.136 35.838 15.229 1.00 30.40 50.100 36.593 16.555 1.00 37.97
	ATOM	585 CG LYS 234 586 CD LYS 234	49.151 35.947 17.569 1.00 53.64
25	ATOM	586 CD L1S 234 587 CE LYS 234	47.694 35.958 17.101 1.00 59.60
35	ATOM ATOM	588 NZ LYS 234	46.773 35.268 18.060 1.00 54.22
	ATOM	589 C LYS 234	50.388 33.686 13.978 1.00 30.35
	ATOM	590 O LYS 234	49.318 33.142 13.716 1.00 32.50
	ATOM	591 N LYS 235	51.425 33.687 13.144 1.00 23.98
40	ATOM	592 CA LYS 235	51.351 33.071 11.828 1.00 22.75
40	ATOM	593 CB LYS 235	52.353 33.737 10.896 1.00 23.12
	ATOM	594 CG LYS 235	51.997 35.181 10.631 1.00 20.88
	ATOM	595 CD LYS 235	52.982 35.836 9.688 1.00 26.50
	ATOM	596 CE LYS 235	52.512 37.227 9.310 1.00 31.33
45	ATOM	597 NZ LYS 235	53.439 37.862 8.341 1.00 36.51
	ATOM	598 C LYS 235	51.508 31.554 11.791 1.00 28.37
	ATOM	599 O LYS 235	51.491 30.948 10.721 1.00 29.62
	ATOM	600 N LEU 236	51.700 30.943 12.954 1.00 33.22
	ATOM	601 CA LEU 236	51.828 29.494 13.036 1.00 32.24
50	ATOM	602 CB LEU 236	52.911 29.101 14.043 1.00 26.25

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603 CG LEU 236
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            604 CD1 LEU 236
                                55.289 29.113 14.806 1.00 20.52
    ATOM
                                54.750 29.054 12.374 1.00 20.29
            605 CD2 LEU 236
    ATOM
                               50.470 28.984 13.502 1.00 37.08
    ATOM
            606 C LEU 236
                               50.013 29.342 14.588 1.00 34.23
    ATOM
            607 O LEU 236
                               49.811 28.134 12.695 1.00 44.89
            608 N PRO 237
    ATOM
                                50.351 27.597 11.432 1.00 42.95
            609 CD PRO 237
    ATOM
                                48.491 27.556 12.990 1.00 48.88
            610 CA PRO 237
    ATOM
                                48.396 26.406 11.987 1.00 51.40
            611 CB PRO 237
    ATOM
                                49.142 26.931 10.813 1.00 53.54
            612 CG PRO 237
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    ATOM
            613 C PRO 237
                               48.278 27.072 14.430 1.00 49.12
    ATOM
                               47.387 27.551 15.133 1.00 48.18
            614 O PRO 237
    ATOM
            615 N MET 238
                                49.104 26.126 14.860 1.00 45.79
    ATOM
                                49.029 25.558 16.200 1.00 52.79
    ATOM
            616 CA MET 238
            617 CB MET 238
                                50.133 24.505 16.378 1.00 49.72
     ATOM
15
            618 CG MET 238
619 SD MET 238
                                49.861 23.195 15.637 1.00 58.16
     ATOM
                                51.342 22.205 15.284 1.00 60.11
    ATOM
                                50.993 21.626 13.625 1.00 53.03
     ATOM
             620 CE MET 238
                                49.103 26.593 17.324 1.00 53.36
             621 C MET 238
     ATOM
                                48.583 26.365 18.420 1.00 58.87
            622 O MET 238
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     ATOM
                               49.713 27.742 17.043 1.00 48.09
            623 N PHE 239
     ATOM
                                49.861 28.793 18.045 1.00 41.38
            624 CA PHE 239
     ATOM
            625 CB PHE 239
                                51.011 29.736 17.677 1.00 32.92
     ATOM
                                51.307 30.763 18.734 1.00 31.32
     ATOM
            626 CG PHE 239
             627 CD1 PHE 239
                                52.162 30.462 19.790 1.00 28.28
25
     ATOM
                                50.715 32.024 18.689 1.00 24.80
             628 CD2 PHE 239
     ATOM
                                52.425 31.402 20.790 1.00 29.45
     ATOM
             629 CE1 PHE 239
                                50.970 32.973 19.682 1.00 32.29
     ATOM
             630 CE2 PHE 239
                                51.828 32.659 20.737 1.00 26.00
     ATOM
             631 CZ PHE 239
             632 C PHE 239
                               48.590 29.592 18.344 1.00 37.40
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                               48.194 29.696 19.501 1.00 33.32
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             633 O PHE 239
                               47.958 30.166 17.321 1.00 36.32
     ATOM
             634 N SER 240
                                46.745 30.959 17.529 1.00 39.00
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             635 CA SER 240
     ATOM
             636 CB SER 240
                                46.385 31.724 16.258 1.00 47.52
                                47.390 32.671 15.947 1.00 52.67
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             637 OG SER 240
                               45.539 30.158 18.032 1.00 36.82
             638 C SER 240
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                               44.548 30.743 18.485 1.00 43.02
             639 O SER 240
     ATOM
                                45.617 28.833 17.931 1.00 38.98
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             640 N GLU 241
     ATOM
             641 CA GLU 241
                                44.554 27.954 18.408 1.00 40.35
             642 CB GLU 241
                                44.788 26.521 17.926 1.00 49.38
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     ATOM
                                44.541 26.287 16.452 1.00 65.25
     ATOM
             643 CG GLU 241
                                44.873 24.856 16.002 1.00 70.72
     ATOM
             644 CD GLU 241
                                 44.806 23.923 16.845 1.00 73.36
     ATOM
             645 OE1 GLU 241
                                 45.211 24.679 14.805 1.00 68.60
     ATOM
             646 OE2 GLU 241
                                44.550 27.968 19.934 1.00 37.83
             647 C GLU 241
45
     ATOM
                                43.504 27.857 20.570 1.00 40.77
     ATOM
             648 O GLU 241
                                45.747 28.103 20.498 1.00 34.71
     ATOM
             649 N LEU 242
                                45.974 28.132 21.944 1.00 31.77
     ATOM
             650 CA LEU 242
             651 CB LEU 242
                                47.478 28.240 22.215 1.00 24.87
     ATOM
             652 CG LEU 242
                                48.345 27.006 22.455 1.00 30.51
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     ATOM
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47.814 25.763 21.772 1.00 31.72
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            653 CD1 LEU 242
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    ATOM
            654 CD2 LEU 242
                               45.274 29.287 22.657 1.00 29.41
            655 C LEU 242
    ATOM
            656 O LEU 242
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            657 N PRO 243
                               44.913 29.089 23.938 1.00 32.37
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                               44.976 27.849 24.728 1.00 27.94
            658 CD PRO 243
    ATOM
                               44.253 30.165 24.685 1.00 33.92
            659 CA PRO 243
    ATOM
                               44.041 29.537 26.065 1.00 29.41
            660 CB PRO 243
    ATOM
                               43.929 28.072 25.775 1.00 30.77
            661 CG PRO 243
    ATOM
           662 C PRO 243
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                               46.461 31.110 24.809 1.00 38.79
            663 O PRO 243
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                               44.751 32.570 24.834 1.00 39.67
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                               45.621 33.749 24.931 1.00 45.78
            665 CA CYS 244
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                               44.788 35.028 25.102 1.00 71.13
    ATOM
            666 CB CYS 244
                               44.068 35.680 23.580 1.00100.76
    ATOM
            667 SG CYS 244
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            669 C CYS 244
                               46.660 33.665 26.051 1.00 40.08
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            670 O CYS 244
                               47.797 34.096 25.879 1.00 35.68
    ATOM
                               46.265 33.088 27.184 1.00 34.25
    ATOM
            671 N GLU 245
                                47.156 32.939 28.337 1.00 34.60
            672 CA GLU 245
     ATOM
                                46.426 32.296 29.524 1.00 42.20
            673 CB GLU 245
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                                45.356 33.171 30.160 1.00 41.92
            674 CG GLU 245
     ATOM
                                43.947 32.808 29.730 1.00 39.68
    ATOM 675 CD GLU 245
     ATOM 676 OE1 GLU 245
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                                43.697 32.644 28.516 1.00 48.13
     ATOM 677 OE2 GLU 245
    ATOM 678 C GLU 245
                               48.376 32.109 27.984 1.00 29.54
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            679 O GLU 245
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                               48.146 31.034 27.236 1.00 26.40
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            680 N ASP 246
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            681 CA ASP 246
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                               48.650 28.887 26.153 1.00 29.86
            682 CB ASP 246
     ATOM
                               48.184 27.876 27.175 1.00 34.10
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     ATOM
            683 CG ASP 246
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     ATOM
            684 OD1 ASP 246
     ATOM
            685 OD2 ASP 246
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            686 C ASP 246
                               50.103 30.875 25.790 1.00 28.07
                               51.331 30.789 25.863 1.00 27.35
     ATOM
            687 O ASP 246
     ATOM 688 N GLN 247
                               49.472 31.577 24.851 1.00 25.53
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            689 CA GLN 247
                                50.198 32.327 23.829 1.00 26.08
     ATOM
            690 CB GLN 247
                                49.228 33.089 22.924 1.00 23.38
     ATOM
            691 CG GLN 247
                                48.303 32.213 22.091 1.00 23.76
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                                47.429 33.029 21.151 1.00 26.89
            692 CD GLN 247
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                                47.853 34.054 20.628 1.00 33.51
            693 OE1 GLN 247
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                                46.198 32.593 20.957 1.00 27.44
     ATOM 694 NE2 GLN 247
                               51.133 33.313 24.511 1.00 22.74
            695 C GLN 247
     ATOM
                               52.326 33.373 24.205 1.00 27.63
            696 O GLN 247
     ATOM
                              50.588 34.047 25.473 1.00 25.03
            697 N ILE 248
     ATOM
                               51.353 35.035 26.220 1.00 25.94
     ATOM
            698 CA ILE 248
45
                               50.436 35.781 27.226 1.00 24.84
            699 CB ILE 248
     ATOM
                               51.251 36.633 28.179 1.00 21.87
            700 CG2 ILE 248
     ATOM
            701 CG1 ILE 248
                               49.430 36.652 26.459 1.00 27.98
     ATOM
                               48.359 37.298 27.328 1.00 29.90
            702 CD1 ILE 248
     ATOM
                              52.535 34.382 26.939 1.00 27.53
            703 C ILE 248
50
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	ATOM	704 O ILE 248	53.671 34.847 26.833 1.00 29.35
	ATOM	705 N ILE 249	52.279 33.274 27.622 1.00 24.38
	ATOM	706 CA ILE 249	53.334 32.582 28.354 1.00 26.26
	ATOM	707 CB ILE 249	52.759 31.395 29.166 1.00 29.81
5	ATOM	708 CG2 ILE 249	53.874 30.521 29.726 1.00 29.16
	ATOM	709 CG1 ILE 249	51.883 31.923 30.300 1.00 27.15
	ATOM	710 CD1 ILE 249	51.173 30.838 31.076 1.00 32.35
	ATOM	711 C ILE 249	54.448 32.103 27.422 1.00 27.78
	ATOM	712 O ILE 249	55.634 32.297 27.708 1.00 29.37
10	ATOM	713 N LEU 250	54.061 31.516 26.289 1.00 29.25
	ATOM	714 CA LEU 250	55.021 31.005 25.319 1.00 24.49
	ATOM	715 CB LEU 250	54.303 30.224 24.214 1.00 23.75
	ATOM	716 CG LEU 250	53.541 28.962 24.629 1.00 23.18
	ATOM	717 CD1 LEU 250	52.886 28.353 23.416 1.00 19.94
15	ATOM	718 CD2 LEU 250	54.475 27.960 25.278 1.00 20.76
	ATOM	719 C LEU 250	55.878 32.116 24.714 1.00 22.20
	ATOM	720 O LEU 250	57.082 31.940 24.528 1.00 23.49
	ATOM	721 N LEU 251	55.256 33.249 24.399 1.00 24.21
	ATOM	722 CA LEU 251	55.980 34.384 23.831 1.00 27.98
20	ATOM	723 CB LEU 251	55.010 35.488 23.408 1.00 25.91
	ATOM	724 CG LEU 251	54.287 35.245 22.085 1.00 29.46
	ATOM	725 CD1 LEU 251	53.121 36.217 21.939 1.00 35.03
	ATOM	726 CD2 LEU 251	55.268 35.364 20.924 1.00 23.65
	ATOM	727 C LEU 251	56.998 34.931 24.828 1.00 26.85
25	ATOM	728 O LEU 251	58.165 35.143 24.484 1.00 23.12
	ATOM	729 N LYS 252	56.556 35.145 26.063 1.00 25.33
	ATOM	730 CA LYS 252	57.427 35.644 27.119 1.00 31.33
	ATOM	731 CB LYS 252	56.659 35.723 28.437 1.00 37.06
20	ATOM	732 CG LYS 252	55.593 36.805 28.511 1.00 41.75 54.779 36.619 29.783 1.00 52.64
30	ATOM	733 CD LYS 252 734 CE LYS 252	54.779 36.619 29.783 1.00 52.64 53.822 37.767 30.057 1.00 62.60
	ATOM ATOM	734 CE L1S 232 735 NZ LYS 252	54.503 39.005 30.520 1.00 71.68
	ATOM	736 C LYS 252	58.622 34.705 27.293 1.00 29.08
	ATOM	730 C L13 252 737 O LYS 252	59.758 35.150 27.460 1.00 35.24
35	ATOM	737 O L13 232 738 N GLY 253	58.355 33.403 27.211 1.00 24.98
33	ATOM	739 CA GLY 253	59.407 32.416 27.369 1.00 22.80
	ATOM	740 C GLY 253	60.413 32.282 26.235 1.00 26.90
	ATOM	741 O GLY 253	61.572 31.948 26.489 1.00 31.90
	ATOM	742 N CYS 254	60.013 32.574 24.997 1.00 25.42
40	ATOM	743 CA CYS 254	60.932 32.427 23.863 1.00 20.71
	ATOM	744 CB CYS 254	60.314 31.509 22.811 1.00 24.98
	ATOM	745 SG CYS 254	58.976 32.310 21.909 1.00 24.24
	ATOM	746 C CYS 254	61.353 33.716 23.164 1.00 22.79
	ATOM	747 O CYS 254	62.217 33.683 22.282 1.00 23.23
45	ATOM	748 N CYS 255	60.757 34.842 23.539 1.00 21.47
	ATOM	749 CA CYS 255	61.061 36.114 22.884 1.00 22.50
	ATOM	750 CB CYS 255	60.318 37.262 23.567 1.00 21.72
	ATOM	751 SG CYS 255	60.353 38.768 22.597 1.00 24.73
	ATOM	752 C CYS 255	62.547 36.457 22.738 1.00 23.81
50	ATOM	753 O CYS 255	63.015 36.746 21.632 1.00 23.48

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63.294 36.402 23.838 1.00 22.13
             754 N MET 256
     ATOM
                                64.719 36.713 23.792 1.00 22.91
    ATOM
             755 CA MET 256
                                65.286 36.810 25.213 1.00 23.78
     ATOM
             756 CB MET 256
                                66.781 37.094 25.272 1.00 17.41
             757 CG MET 256
     ATOM
                                67.196 38.632 24.415 1.00 23.65
             758 SD MET 256
     ATOM
                                69.010 38.715 24.624 1.00 18.57
             759 CE MET 256
     ATOM
                               65.487 35.671 22.980 1.00 21.41
             760 C MET 256
     ATOM
             761 O MET 256
                                66.432 36.005 22.260 1.00 22.01
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             762 N GLU 257
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     ATOM
                                65.705 33.323 22.345 1.00 22.90
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             763 CA GLU 257
                                65.085 31.989 22.753 1.00 24.00
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     ATOM
             765 CG GLU 257
                                65.522 31.521 24.125 1.00 33.44
                                64.564 30.527 24.735 1.00 38.03
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                                 63.977 29.705 24.000 1.00 45.59
             767 OE1 GLU 257
     ATOM
             768 OE2 GLU 257
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             769 C GLU 257
                               65,595 33,526 20.840 1.00 21.68
     ATOM
                               66.586 33.421 20.107 1.00 20.02
             770 O GLU 257
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                               64.383 33.852 20.391 1.00 17.07
     ATOM
             771 N ILE 258
             772 CA ILE 258
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             773 CB ILE 258
                               62.613 34.207 18.684 1.00 17.33
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     ATOM
             774 CG2 ILE 258
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                                61.952 32.831 18.885 1.00 16.69
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     ATOM
                                60.450 32.783 18.632 1.00 16.31
             776 CD1 ILE 258
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                               64,911 35.324 18.501 1.00 17.65
     ATOM
             777 C ILE 258
                               65.605 35.263 17.484 1.00 22.58
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             778 O ILE 258
             779 N MET 259
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     ATOM
                                 65.584 37.628 18.909 1.00 15.03
             780 CA MET 259
     ATOM
             781 CB MET 259
                                 65,234 38,771 19,856 1,00 20,12
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             782 CG MET 259
                                 63.791 39.191 19.775 1.00 17.19
     ATOM
                                63.523 40.795 20.524 1.00 28.92
             783 SD MET 259
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     ATOM
                                63.718 40.406 22.261 1.00 19.58
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             784 CE MET 259
                                67.090 37.402 18.884 1.00 18.84
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             785 C MET 259
                                67.783 37.912 17.996 1.00 29.07
             786 O MET 259
     ATOM
                               67.590 36.618 19.837 1.00 21.45
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     ATOM
                                69.019 36.319 19.906 1.00 18.71
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                                69.128 36.421 22.329 1.00 25.42
             790 OG SER 260
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                               69.430 35.469 18.709 1.00 17.83
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             792 O SER 260
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                                67.739 32.608 17.053 1.00 22.66
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             795 CB LEU 261
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     ATOM
             797 CD1 LEU 261
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     ATOM
             798 CD2 LEU 261
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             799 C LEU 261
                               69.779 34.402 15.091 1.00 22.62
             800 O LEU 261
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             801 N ARG 262
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     ATOM
             802 CA ARG 262
                                 67.816 36.301 14.643 1.00 25.32
                                 66.525 37.115 14.677 1.00 21.95
     ATOM
             803 CB ARG 262
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65.304 36.268 14.362 1.00 21.48
             804 CG ARG 262
     ATOM
                                64.026 37.077 14.345 1.00 19.12
             805 CD ARG 262
     ATOM
                                62.990 36.377 13.599 1.00 22.18
             806 NE ARG 262
     ATOM
                                61.780 36.862 13.333 1.00 22.88
     ATOM
             807 CZ ARG 262
                                 61.429 38.075 13.752 1.00 20.81
    ATOM
            808 NH1 ARG 262
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            809 NH2 ARG 262
     ATOM
                               69.044 37.196 14.531 1.00 25.05
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            811 O ARG 262
                               69.485 37.513 13.427 1.00 22.98
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     ATOM
            814 CB ALA 263
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                               72.026 37.514 15.368 1.00 25.21
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            815 C ALA 263
            816 O ALA 263
                               72.825 37.844 14.492 1.00 31.14
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             818 CA ALA 264
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            820 C ALA 264
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                               74.460 34.773 13.886 1.00 25.66
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            823 CA VAL 265
     ATOM
            824 CB VAL 265
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            825 CG1 VAL 265
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     ATOM
            826 CG2 VAL 265
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            843 CG TYR 267
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             845 CE1 TYR 267
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             846 CD2 TYR 267
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             847 CE2 TYR 267
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             848 CZ TYR 267
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             849 OH TYR 267
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                               78.319 38.769 11.239 1.00 44.62
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                               79.248 38.963 10.133 1.00 45.56
            853 CA ASP 268
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            855 CG ASP 268
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                                80.204 39.755 7.502 1.00 55.65
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            856 OD1 ASP 268
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            857 OD2 ASP 268
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            883 OD2 ASP 272
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            888 CB THR 273
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                               77.168 41.757 14.993 1.00 36.08
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            896 CG LEU 274
                                75.310 39.472 18.444 1.00 26.29
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            897 CD1 LEU 274
                                75.744 38.237 16.309 1.00 27.43
            898 CD2 LEU 274
     ATOM
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            900 O LEU 274
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            902 CA THR 275
     ATOM
                                72.773 42.522 11.556 1.00 36.04
            903 CB THR 275
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	A TO 1 4	904 OG1 THR 275	74.028 42.625 10.875 1.00 41.52
	ATOM	904 OG1 THR 275 905 CG2 THR 275	71.852 43.583 11.008 1.00 36.47
	ATOM		71.673 42.655 13.814 1.00 34.32
	ATOM		71.055 41.590 13.907 1.00 34.96
_	ATOM	907 O THR 275 908 N LEU 276	71.292 43.767 14.432 1.00 31.79
5	ATOM		70.044 43.840 15.173 1.00 29.47
	ATOM	909 CA LEU 276	70.181 44.766 16.389 1.00 25.29
	ATOM	910 CB LEU 276	71.328 44.501 17.383 1.00 29.01
	ATOM	911 CG LEU 276	
	ATOM	912 CD1 LEU 276	
10	ATOM	913 CD2 LEU 276	71.358 43.042 17.834 1.00 22.79
	ATOM	914 C LEU 276	68.966 44.350 14.228 1.00 31.69
	ATOM	915 O LEU 276	69.175 45.335 13.510 1.00 33.87
	ATOM	916 N SER 277	67.862 43.608 14.162 1.00 33.07
	ATOM	917 CA SER 277	66.721 43.935 13.315 1.00 30.61
15	ATOM	918 CB SER 277	65.949 45.111 13.909 1.00 22.87
	ATOM	919 OG SER 277	65.587 44.822 15.250 1.00 23.35
	ATOM	920 C SER 277	67.103 44.200 11.860 1.00 31.85
	ATOM	921 O SER 277	66.433 44.958 11.158 1.00 32.13
	ATOM	922 N GLY 278	68.188 43.566 11.421 1.00 32.29
20	ATOM	923 CA GLY 278	68.664 43.716 10.058 1.00 37.59
	ATOM	924 C GLY 278	69.063 45.122 9.639 1.00 43.26
	ATOM	925 O GLY 278	69.313 45.358 8.455 1.00 42.60
	ATOM	926 N GLU 279	69.177 46.038 10.599 1.00 43.42
	ATOM	927 CA GLU 279	69.532 47.420 10.291 1.00 44.55
25	ATOM	928 CB GLU 279	68.292 48.310 10.394 1.00 44.66
	ATOM	929 CG GLU 279	67.671 48.344 11.783 1.00 54.19
	ATOM	930 CD GLU 279	66.400 49.171 11.845 1.00 64.96
	ATOM	931 OE1 GLU 279	65.627 49.174 10.859 1.00 71.43
	ATOM	932 OE2 GLU 279	66.167 49.814 12.891 1.00 66.65
30	ATOM	933 C GLU 279	70.654 48.019 11.133 1.00 45.52
	ATOM	934 O GLU 279	71.207 49.057 10.772 1.00 51.83
	ATOM	935 N MET 280	71.007 47.373 12.242 1.00 44.66
	ATOM	936 CA MET 280	72.060 47.904 13.105 1.00 34.22
	ATOM	937 CB MET 280	71.470 48.382 14.433 1.00 32.38
35	ATOM	938 CG MET 280	72.479 49.058 15.345 1.00 37.87
	ATOM	939 SD MET 280	71.912 49.201 17.052 1.00 41.78
	ATOM	940 CE MET 280	70.650 50.495 16.911 1.00 37.01
	ATOM	941 C MET 280	73.183 46.920 13.386 1.00 35.70
	ATOM	942 O MET 280	72.976 45.900 14.044 1.00 36.99
40	ATOM	943 N ALA 281	74.366 47.221 12.867 1.00 34.80
	ATOM	944 CA ALA 281	75.535 46.377 13.091 1.00 35.11
	ATOM	945 CB ALA 281	76.529 46.527 11.955 1.00 31.27
	ATOM	946 C ALA 281	76.155 46.837 14.406 1.00 35.96
	ATOM	947 O ALA 281	76.478 48.015 14.570 1.00 39.10
45	ATOM	948 N VAL 282	76.285 45.916 15.353 1.00 36.46
	ATOM	949 CA VAL 282	76.839 46.246 16.655 1.00 36.05
	ATOM	950 CB VAL 282	75.783 46.090 17.783 1.00 35.60
	ATOM	951 CG1 VAL 282	74.633 47.069 17.568 1.00 38.73
	ATOM	952 CG2 VAL 282	75.262 44.660 17.844 1.00 33.27
50	ATOM	953 C VAL 282	78.062 45.408 16.996 1.00 37.70

	ATOM	954 O VAL 282	78.137 44.223 16.660 1.00 37.45
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	ATOM	956 CA ALA 283	80.254 45.375 18.048 1.00 43.73
	ATOM	957 CB ALA 283	81.433 46.352 18.047 1.00 42.04
5	ATOM	958 C ALA 283	80.060 44.752 19.435 1.00 43.28
	ATOM	959 O ALA 283	79.179 45.157 20.203 1.00 45.77
	ATOM	960 N ARG 284	80.903 43.774 19.744 1.00 41.96
	ATOM	961 CA ARG 284	80.866 43.044 21.004 1.00 44.87
	ATOM	962 CB ARG 284	82.084 42.125 21.087 1.00 46.34
10	ATOM	963 CG ARG 284	81.930 40.947 22.017 1.00 51.85
	ATOM	964 CD ARG 284	83.107 40.010 21.844 1.00 60.73
	ATOM	965 NE ARG 284	83.262 39.571 20.455 1.00 54.30
	ATOM	966 CZ ARG 284	83.221 38.300 20.074 1.00 53.66
	ATOM	967 NH1 ARG 284	83.032 37.343 20.973 1.00 49.99
15	ATOM	968 NH2 ARG 284	83.379 37.984 18.797 1.00 47.31
	ATOM	969 C ARG 284	80.803 43.945 22.237 1.00 44.85
	ATOM	970 O ARG 284	79.896 43.806 23.062 1.00 48.26
	ATOM	971 N GLU 285	81.750 44.873 22.349 1.00 41.60
	ATOM	972 CA GLU 285	81.802 45.787 23.484 1.00 41.17
20	ATOM	973 CB GLU 285	83.043 46.675 23.392 1.00 39.97
	ATOM	974 C GLU 285	80.538 46.640 23.603 1.00 40.08
	ATOM	975 O GLU 285	80.023 46.849 24.703 1.00 41.16
	ATOM	976 N GLN 286	80.017 47.088 22.463 1.00 38.49
	ATOM	977 CA GLN 286	78.818 47.926 22.425 1.00 36.25
25	ATOM	978 CB GLN 286	78.549 48.401 20.997 1.00 39.50
	ATOM	979 CG GLN 286	79.619 49.311 20.424 1.00 43.62
	ATOM	980 CD GLN 286	79.324 49.710 18.987 1.00 49.48
	ATOM	981 OE1 GLN 286	79.253 48.856 18.097 1.00 48.41
	ATOM	982 NE2 GLN 286	79.125 51.000 18.755 1.00 47.15
30	ATOM	983 C GLN 286	77.563 47.255 22.988 1.00 35.40
	ATOM	984 O GLN 286	76.903 47.806 23.871 1.00 31.24
	ATOM	985 N LEU 287	77.234 46.071 22.480 1.00 32.96
	ATOM	986 CA LEU 287	76.055 45.349 22.950 1.00 33.40
	ATOM	987 CB LEU 287	75.767 44.138 22.054 1.00 28.67
35	ATOM	988 CG LEU 287	74.466 43.375 22.342 1.00 26.66
	ATOM	989 CD1 LEU 287	73.263 44.305 22.244 1.00 19.41
	ATOM	990 CD2 LEU 287	74.325 42.221 21.368 1.00 24.84
	ATOM	991 C LEU 287	76.234 44.914 24.406 1.00 34.81
	ATOM	992 O LEU 287	75.265 44.857 25.175 1.00 33.92
40	ATOM	993 N LYS 288	77.476 44.621 24.781 1.00 35.38
	ATOM	994 CA LYS 288	77.814 44.204 26.140 1.00 36.12
	ATOM	995 CB LYS 288	79.296 43.839 26.210 1.00 37.13
	ATOM	996 CG LYS 288	79.762 43.280 27.533 1.00 44.61
	ATOM	997 CD LYS 288	81.256 43.018 27.494 1.00 54.07
45	ATOM	998 CE LYS 288	81.757 42.435 28.801 1.00 60.87
	ATOM	999 NZ LYS 288	81.291 41.041 29.039 1.00 61.53
	ATOM	1000 C LYS 288	77.510 45.345 27.109 1.00 36.90
	ATOM	1001 O LYS 288	76.684 45.206 28.013 1.00 40.68
	ATOM	1002 N ASN 289	78.129 46.495 26.863 1.00 35.94
50	ATOM	1003 CA ASN 289	77.947 47.680 27.695 1.00 36.12
-			

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ATOM 1004 CB ASN 289
                                78.982 48.738 27.332 1.00 31.78
    ATOM 1005 CG ASN 289
                                80.388 48.263 27.569 1.00 40.31
    ATOM 1006 OD1 ASN 289
                                 80.627 47.422 28.440 1.00 43.12
                                 81.326 48.758 26.775 1.00 35.36
    ATOM 1007 ND2 ASN 289
                               76.553 48.277 27.590 1.00 36.98
    ATOM 1008 C ASN 289
5
                               76.099 48.959 28.509 1.00 34.29
    ATOM 1009 O ASN 289
                               75.883 48.032 26.466 1.00 32.65
    ATOM 1010 N GLY 290
                                74.541 48.550 26.256 1.00 28.61
    ATOM 1011 CA GLY 290
                               73.497 48.001 27.210 1.00 26.54
    ATOM 1012 C GLY 290
    ATOM 1013 O GLY 290
                               72.362 48.480 27.234 1.00 31.06
10
    ATOM 1014 N GLY 291
                               73.861 46.978 27.977 1.00 28.89
                                72.929 46.413 28.937 1.00 25.24
    ATOM 1015 CA GLY 291
                               72.872 44.900 28.997 1.00 28.12
    ATOM 1016 C GLY 291
    ATOM 1017 O GLY 291
                               72.335 44.345 29.955 1.00 31.16
                               73.406 44.223 27.985 1.00 29.51
    ATOM 1018 N LEU 292
15
                                73.361 42.766 27.969 1.00 32.79
    ATOM 1019 CA LEU 292
                                73.304 42.240 26.531 1.00 28.00
    ATOM 1020 CB LEU 292
                                71.948 42.355 25.827 1.00 23.68
    ATOM 1021 CG LEU 292
                                72.004 41.626 24.509 1.00 26.12
    ATOM 1022 CD1 LEU 292
                                 70.851 41.764 26.694 1.00 23.36
    ATOM 1023 CD2 LEU 292
20
                               74.484 42.085 28.742 1.00 32.33
     ATOM 1024 C LEU 292
                               74.312 40.967 29.232 1.00 32.22
     ATOM 1025 O LEU 292
    ATOM 1026 N GLY 293
ATOM 1027 CA GLY 293
                                75.627 42.750 28.846 1.00 30.31
                                76.751 42.176 29.561 1.00 28.82
                                77.238 40.894 28.913 1.00 29.87
     ATOM 1028 C GLY 293
25
                                77.432 40.843 27.698 1.00 35.43
     ATOM 1029 O GLY 293
                                77.392 39.848 29.714 1.00 31.88
     ATOM 1030 N VAL 294
                                77.866 38.561 29.217 1.00 35.77
     ATOM 1031 CA VAL 294
                                78.232 37.590 30.363 1.00 34.29
     ATOM 1032 CB VAL 294
     ATOM 1033 CG1 VAL 294
                                 79.462 38.092 31.095 1.00 37.54
30
                                 77.065 37.425 31.322 1.00 25.62
     ATOM 1034 CG2 VAL 294
     ATOM 1035 C VAL 294
                                76.882 37.879 28.274 1.00 35.89
                                77.263 36.960 27.541 1.00 37.99
     ATOM 1036 O VAL 294
     ATOM 1037 N VAL 295
                                75.619 38.304 28.305 1.00 34.41
                                74.616 37.728 27.413 1.00 32.98
     ATOM 1038 CA VAL 295
35
                                73.208 38.298 27.677 1.00 31.25
     ATOM 1039 CB VAL 295
                                 72.208 37.706 26.694 1.00 23.54
     ATOM 1040 CG1 VAL 295
                                 72.783 37.993 29.101 1.00 23.07
     ATOM 1041 CG2 VAL 295
                                75.057 38.062 25.993 1.00 33.92
     ATOM 1042 C VAL 295
                                74.932 37.238 25.090 1.00 36.95
     ATOM 1043 O VAL 295
40
                                75.625 39.253 25.820 1.00 31.27
     ATOM 1044 N SER 296
                                76.118 39.695 24.521 1.00 33.38
     ATOM 1045 CA SER 296
                                76.667 41.115 24.620 1.00 24.78
     ATOM 1046 CB SER 296
                                77.368 41.478 23.449 1.00 25.43
     ATOM 1047 OG SER 296
     ATOM 1048 C SER 296
                               77.216 38.748 24.045 1.00 35.86
45
                                77.220 38.324 22.886 1.00 39.60
     ATOM 1049 O SER 296
                                78.135 38.402 24.943 1.00 37.41
     ATOM 1050 N ASP 297
                                79.227 37.490 24.602 1.00 35.39
     ATOM 1051 CA ASP 297
                                80.147 37.269 25.808 1.00 43.07
     ATOM 1052 CB ASP 297
     ATOM 1053 CG ASP 297
                                80.839 38.540 26.266 1.00 45.07
50
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	ATOM	1054 OD1 ASP 297	81.175 39.398 25.419 1.00 48.02
	ATOM	1055 OD2 ASP 297	81.064 38.670 27.485 1.00 50.13
	ATOM	1056 C ASP 297	78.662 36.145 24.161 1.00 30.87
	ATOM	1057 O ASP 297	79.155 35.534 23.213 1.00 33.92
5	ATOM	1058 N ALA 298	77.625 35.698 24.861 1.00 28.96
	ATOM	1059 CA ALA 298	76.971 34.428 24.574 1.00 30.60
	ATOM	1060 CB ALA 298	75.889 34.157 25.610 1.00 27.56
	ATOM	1061 C ALA 298	76.377 34.408 23.163 1.00 33.04
	ATOM	1062 O ALA 298	76.538 33.426 22.426 1.00 32.48
10	ATOM	1063 N ILE 299	75.706 35.493 22.786 1.00 30.92
	ATOM	1064 CA ILE 299	75.091 35.588 21.468 1.00 24.71
	ATOM	1065 CB ILE 299	74.138 36.789 21.368 1.00 22.98
	ATOM	1066 CG2 ILE 299	73.430 36.786 20.018 1.00 21.90
	ATOM	1067 CG1 ILE 299	73.091 36.707 22.477 1.00 20.91
15	ATOM	1068 CD1 ILE 299	72.266 37.951 22.634 1.00 19.86
13	ATOM	1069 C ILE 299	76.168 35.680 20.395 1.00 26.77
	ATOM	1070 O ILE 299	76.036 35.069 19.335 1.00 30.21
	ATOM	1070 O IEE 233	77.238 36.428 20.673 1.00 29.08
	ATOM	1072 CA PHE 300	78.345 36.562 19.726 1.00 28.06
20	ATOM	1072 CR THE 300	79.386 37.565 20.235 1.00 29.06
20	ATOM	1074 CG PHE 300	79.289 38.920 19.590 1.00 28.14
	ATOM	1074 CO THE 300	78.449 39.896 20.113 1.00 27.20
	ATOM	1075 CD1111E 300	80.017 39.209 18.437 1.00 29.11
	ATOM	1070 CE1 PHE 300	78.332 41.139 19.499 1.00 28.18
25	ATOM	1077 CE1THE 300	79.908 40.450 17.815 1.00 29.07
23	ATOM	1079 CZ PHE 300	79.064 41.416 18.348 1.00 22.61
	ATOM	1080 C PHE 300	78.991 35.201 19.485 1.00 29.00
	ATOM	1081 O PHE 300	79.278 34.833 18.344 1.00 30.35
	ATOM	1082 N GLU 301	79.183 34.442 20.560 1.00 31.81
30	ATOM	1083 CA GLU 301	79.767 33.111 20.470 1.00 34.96
30	ATOM	1084 CB GLU 301	79.962 32.528 21.865 1.00 30.78
	ATOM	1085 C GLU 301	78.850 32.210 19.634 1.00 35.49
	ATOM	1086 O GLU 301	79.322 31.438 18.793 1.00 35.76
	ATOM	1087 N LEU 302	77.543 32.313 19.869 1.00 32.14
35	ATOM	1088 CA LEU 302	76.559 31.522 19.132 1.00 25.56
	ATOM	1089 CB LEU 302	75.147 31.760 19.682 1.00 23.33
	ATOM	1090 CG LEU 302	73.992 31.006 19.010 1.00 28.73
	ATOM	1091 CD1 LEU 302	74.093 29.509 19.270 1.00 23.93
	ATOM	1092 CD2 LEU 302	72.667 31.551 19.514 1.00 21.32
40		1093 C LEU 302	76.617 31.885 17.650 1.00 23.10
, •	ATOM	1094 O LEU 302	76.664 31.001 16.796 1.00 26.79
	ATOM	1095 N GLY 303	76.672 33.181 17.353 1.00 22.79
	ATOM	1096 CA GLY 303	76,745 33.631 15.974 1.00 21.60
	ATOM	1097 C GLY 303	77.978 33.104 15.256 1.00 30.42
45	ATOM	1098 O GLY 303	77.889 32.619 14.125 1.00 29.18
	ATOM	1090 O GET 303 1099 N ALA 304	79.132 33.182 15.912 1.00 31.15
	ATOM	1100 CA ALA 304	80.375 32.703 15.313 1.00 35.44
	ATOM	1101 CB ALA 304	81.562 32.995 16.235 1.00 29.16
	ATOM	1102 C ALA 304	80.300 31.208 14.978 1.00 35.15
50	ATOM	1103 O ALA 304	80.705 30.785 13.891 1.00 37.13
			

	ATOM	1104 N SER 305	79.753 30.414 15.892 1.00 33.91
	ATOM	1105 CA SER 305	79.638 28.979 15.663 1.00 36.39
	ATOM	1106 CB SER 305	79.395 28.237 16.980 1.00 32.71
	ATOM	1107 OG SER 305	78.265 28.749 17.663 1.00 48.66
5	ATOM	1108 C SER 305	78.558 28.619 14.641 1.00 37.61
-	ATOM	1109 O SER 305	78.747 27.697 13.845 1.00 39.92
	ATOM	1110 N LEU 306	77.443 29.349 14.651 1.00 38.21
	ATOM	1111 CA LEU 306	76.350 29.092 13.714 1.00 35.65
	ATOM	1112 CB LEU 306	75.094 29.894 14.077 1.00 25.49
10	ATOM	1113 CG LEU 306	74.209 29.374 15.212 1.00 26.18
	ATOM	1114 CD1 LEU 306	72.988 30.262 15.361 1.00 23.40
	ATOM	1115 CD2 LEU 306	73.777 27.952 14.921 1.00 23.57
	ATOM	1116 C LEU 306	76.723 29.356 12.258 1.00 38.05
	ATOM	1117 O LEU 306	76.092 28.809 11.353 1.00 37.22
15	ATOM	1118 N SER 307	77.743 30.185 12.030 1.00 40.41
	ATOM	1119 CA SER 307	78.199 30.511 10.677 1.00 40.85
	ATOM	1120 CB SER 307	79.415 31.442 10.736 1.00 37.32
	ATOM	1121 OG SER 307	79.086 32.678 11.344 1.00 56.20
	ATOM	1122 C SER 307	78.550 29.270 9.852 1.00 39.87
20	ATOM	1123 O SER 307	78.221 29.191 8.670 1.00 44.27
	ATOM	1124 N ALA 308	79.207 28.305 10.487 1.00 39.29
	ATOM	1125 CA ALA 308	79.609 27.066 9.826 1.00 33.10
	ATOM	1126 CB ALA 308	80.607 26.310 10.696 1.00 33.37
	ATOM	1127 C ALA 308	78.403 26.177 9.502 1.00 34.07
25	ATOM	1128 O ALA 308	78.467 25.340 8.600 1.00 40.61
	ATOM	1129 N PHE 309	77.305 26.368 10.230 1.00 31.85
	ATOM	1130 CA PHE 309	76.095 25.581 10.015 1.00 35.24
	ATOM	1131 CB PHE 309	75.149 25.698 11.219 1.00 33.69
20	ATOM	1132 CG PHE 309	75.618 24.954 12.437 1.00 36.16 76.785 25.327 13.090 1.00 43.79
30	ATOM	1133 CD1 PHE 309	74.903 23.867 12.922 1.00 38.03
	ATOM	1134 CD2 PHE 309 1135 CE1 PHE 309	77.237 24.627 14.210 1.00 41.12
	ATOM	1135 CE1 PHE 309	75.346 23.161 14.040 1.00 41.08
	ATOM	1136 CE2 PHE 309	76.514 23.543 14.683 1.00 38.37
35	ATOM ATOM	1137 CZ FHE 309	75.361 25.934 8.720 1.00 36.31
33	ATOM	1139 O PHE 309	74.633 25.095 8.173 1.00 37.84
	ATOM	1140 N ASN 310	75.567 27.155 8.225 1.00 35.22
	ATOM	1141 CA ASN 310	74.933 27.625 6.988 1.00 43.66
	ATOM	1142 CB ASN 310	75.536 26.930 5.760 1.00 54.13
40	ATOM	1143 CG ASN 310	
	ATOM	1144 OD1 ASN 310	77.297 28.527 5.412 1.00 74.62
	ATOM	1145 ND2 ASN 310	77.859 26.348 5.352 1.00 68.85
	ATOM	1146 C ASN 310	73.430 27.385 7.013 1.00 38.37
	ATOM	1147 O ASN 310	72.882 26.735 6.123 1.00 36.70
45	ATOM	1148 N LEU 311	72.780 27.865 8.062 1.00 35.22
	ATOM	1149 CA LEU 311	71.345 27.690 8.206 1.00 34.32
	ATOM	1150 CB LEU 311	70.895 28.054 9.630 1.00 30.19
	ATOM	1151 CG LEU 311	71.458 27.306 10.845 1.00 26.76
	ATOM	1152 CD1 LEU 311	70.792 27.847 12.104 1.00 21.37
50	ATOM	1153 CD2 LEU 311	71.217 25.813 10.722 1.00 22.95

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70.601 28.561 7.206 1.00 34.64
    ATOM 1154 C LEU 311
    ATOM 1155 O LEU 311
                               71.087 29.625 6.820 1.00 37.70
    ATOM 1156 N ASP 312
                              69.444 28.091 6.752 1.00 29.40
    ATOM 1157 CA ASP 312
                               68.634 28.867 5.823 1.00 28.65
    ATOM 1158 CB ASP 312
                               68.302 28.061 4.545 1.00 24.79
                               67.459 26.804 4.804 1.00 21.47
    ATOM 1159 CG ASP 312
                                66.994 26.549 5.932 1.00 27.92
    ATOM 1160 OD1 ASP 312
                                67.250 26.057 3.832 1.00 27.53
    ATOM 1161 OD2 ASP 312
                              67.380 29.346 6.557 1.00 25.92
    ATOM 1162 C ASP 312
                              67.167 28.985 7.717 1.00 26.98
    ATOM 1163 O ASP 312
10
                              66.540 30.122 5.878 1.00 21.78
    ATOM 1164 N ASP 313
                               65.315 30.653 6.471 1.00 22.89
    ATOM 1165 CA ASP 313
                               64.517 31.458 5.439 1.00 29.19
    ATOM 1166 CB ASP 313
    ATOM 1167 CG ASP 313
                               65.216 32.739 5.025 1.00 36.82
                                65.985 33.285 5.845 1.00 41.51
    ATOM 1168 OD1 ASP 313
15
    ATOM 1169 OD2 ASP 313
                                64.997 33.203 3.883 1.00 44.19
                              64.421 29.587 7.085 1.00 25.09
    ATOM 1170 C ASP 313
                               63.778 29.829 8.110 1.00 27.60
    ATOM 1171 O ASP 313
                               64.363 28.420 6.449 1.00 20.90
    ATOM 1172 N THR 314
                                63.538 27.322 6.942 1.00 22.71
20
    ATOM 1173 CA THR 314
                               63.408 26.208 5.884 1.00 22.07
    ATOM 1174 CB THR 314
                                62.825 26.746 4.693 1.00 23.15
    ATOM 1175 OG1 THR 314
                                62.542 25.079 6.401 1.00 18.17
    ATOM 1176 CG2 THR 314
                               64.080 26.734 8.249 1.00 19.95
    ATOM 1177 C THR 314
                               63.326 26.477 9.182 1.00 22.40
    ATOM 1178 O THR 314
25
                               65.391 26.536 8.318 1.00 20.01
    ATOM 1179 N GLU 315
                                65.997 25.987 9.523 1.00 19.40
    ATOM 1180 CA GLU 315
    ATOM 1181 CB GLU 315
                                67.454 25.626 9.254 1.00 11.72
                                67.544 24.440 8.322 1.00 13.43
    ATOM 1182 CG GLU 315
                                68.925 24.157 7.791 1.00 18.51
30
     ATOM 1183 CD GLU 315
                                69.666 25.107 7.451 1.00 23.24
    ATOM 1184 OE1 GLU 315
    ATOM 1185 OE2 GLU 315
                                69.254 22.962 7.673 1.00 24.23
    ATOM 1186 C GLU 315
                               65.833 26.960 10.681 1.00 20.12
                               65.425 26.570 11.777 1.00 20.53
     ATOM 1187 O GLU 315
     ATOM 1188 N VAL 316
                               66.055 28.240 10.406 1.00 21.79
35
                                65.898 29.270 11.425 1.00 18.14
    ATOM 1189 CA VAL 316
                                66.346 30.659 10.898 1.00 18.97
     ATOM 1190 CB VAL 316
     ATOM 1191 CG1 VAL 316
                                66.040 31.741 11.929 1.00 19.08
     ATOM 1192 CG2 VAL 316
                                67.840 30.641 10.537 1.00 17.97
                               64,430 29.332 11.880 1.00 22.54
     ATOM 1193 C VAL 316
40
                               64.146 29.433 13.072 1.00 26.47
     ATOM 1194 O VAL 316
                               63.505 29.242 10.924 1.00 19.66
     ATOM 1195 N ALA 317
                                62.076 29.286 11.216 1.00 16.99
     ATOM 1196 CA ALA 317
                                61.279 29.329 9.926 1.00 17.79
     ATOM 1197 CB ALA 317
                               61.619 28.105 12.063 1.00 14.12
     ATOM 1198 C ALA 317
45
                               60.808 28.263 12.970 1.00 17.04
     ATOM 1199 O ALA 317
                               62.104 26.911 11.740 1.00 20.37
     ATOM 1200 N LEU 318
                                61.725 25.714 12.485 1.00 21.12
     ATOM 1201 CA LEU 318
                                62.131 24.448 11.718 1.00 21.80
     ATOM 1202 CB LEU 318
                                61.364 24.265 10.398 1.00 18.11
     ATOM 1203 CG LEU 318
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61.946 23.125 9.594 1.00 16.79
    ATOM 1204 CD1 LEU 318
    ATOM 1205 CD2 LEU 318
                                59.891 24.024 10.676 1.00 12.66
                               62.335 25.752 13.880 1.00 22.03
    ATOM 1206 C LEU 318
    ATOM 1207 O LEU 318
                               61.688 25.373 14.858 1.00 21.35
                               63.564 26.257 13.964 1.00 20.03
    ATOM 1208 N LEU 319
                                64.260 26.395 15.236 1.00 20.24
     ATOM 1209 CA LEU 319
                                65.657 26.960 15.001 1.00 19.07
    ATOM 1210 CB LEU 319
                                66.594 27.108 16.196 1.00 27.61
    ATOM 1211 CG LEU 319
    ATOM 1212 CD1 LEU 319
                                66.518 25.883 17.083 1.00 29.73
                                68.012 27.326 15.699 1.00 20.98
    ATOM 1213 CD2 LEU 319
10
                               63.422 27.334 16.118 1.00 21.16
    ATOM 1214 C LEU 319
                               63.144 27.032 17.279 1.00 26.65
     ATOM 1215 O LEU 319
    ATOM 1216 N GLN 320
                               62.958 28.439 15.539 1.00 20.77
    ATOM 1217 CA GLN 320
                                62.119 29.390 16.265 1.00 17.87
     ATOM 1218 CB GLN 320
                                61.781 30.594 15.388 1.00 18.74
15
                                62.957 31.496 15.111 1.00 21.07
     ATOM 1219 CG GLN 320
                                62.637 32.617 14.150 1.00 22.88
     ATOM 1220 CD GLN 320
                                61.571 32.653 13.528 1.00 26.07
     ATOM 1221 OE1 GLN 320
                                 63.574 33.537 14.006 1.00 20.11
     ATOM 1222 NE2 GLN 320
20
    ATOM 1223 C GLN 320
                               60.829 28.728 16.730 1.00 19.08
     ATOM 1224 O GLN 320
                               60.368 28.976 17.844 1.00 23.39
                               60.251 27.886 15.876 1.00 22.71
     ATOM 1225 N ALA 321
                                59.010 27.187 16.201 1.00 18.86
     ATOM 1226 CA ALA 321
     ATOM 1227 CB ALA 321
                                58.495 26.422 14.993 1.00 17.22
     ATOM 1228 C ALA 321
                               59.220 26.235 17.376 1.00 19.85
25
                               58.362 26.119 18.250 1.00 19.60
     ATOM 1229 O ALA 321
     ATOM 1230 N VAL 322
                               60.368 25.561 17.396 1.00 20.25
                                60.693 24.628 18.469 1.00 21.32
     ATOM 1231 CA VAL 322
     ATOM 1232 CB VAL 322
                                61.956 23.800 18.116 1.00 20.46
     ATOM 1233 CG1 VAL 322
                                 62.418 22.971 19.304 1.00 20.39
30
     ATOM 1234 CG2 VAL 322
                                 61.662 22.890 16.930 1.00 16.83
     ATOM 1235 C VAL 322
                               60.880 25.393 19.785 1.00 20.67
                                60.444 24.941 20.850 1.00 21.28
     ATOM 1236 O VAL 322
                               61.492 26.574 19.701 1.00 21.14
     ATOM 1237 N LEU 323
     ATOM 1238 CA LEU 323
                                61.722 27.417 20.869 1.00 22.94
35
     ATOM 1239 CB LEU 323
                                62.610 28.608 20.511 1.00 16.12
     ATOM 1240 CG LEU 323
                                64.051 28.291 20.115 1.00 22.28
                                64.719 29.532 19.528 1.00 14.87
     ATOM 1241 CD1 LEU 323
                                 64.816 27.750 21.320 1.00 21.55
     ATOM 1242 CD2 LEU 323
                               60.398 27.932 21.410 1.00 22.55
     ATOM 1243 C LEU 323
40
                               60.185 27.986 22.615 1.00 25.21
     ATOM 1244 O LEU 323
                               59.507 28.300 20.502 1.00 24.15
     ATOM 1245 N LEU 324
                                58.200 28.827 20.855 1.00 19.88
     ATOM 1246 CA LEU 324
                                57.499 29.384 19.608 1.00 15.20
     ATOM 1247 CB LEU 324
                                56.067 29.908 19.767 1.00 17.21
     ATOM 1248 CG LEU 324
45
                                 56.021 31.161 20.637 1.00 15.99
     ATOM 1249 CD1 LEU 324
                                 55.496 30.208 18.395 1.00 20.03
     ATOM 1250 CD2 LEU 324
                               57.311 27.795 21.536 1.00 19.83
     ATOM 1251 C LEU 324
     ATOM 1252 O LEU 324
                               56.767 28.064 22.609 1.00 24.47
                                57.197 26.603 20.956 1.00 25.02
     ATOM 1253 N MET 325
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ATOM 1254 CA MET 325
                                56.339 25.563 21.522 1.00 26.72
     ATOM 1255 CB MET 325
                                55.823 24.644 20.410 1.00 30.03
                                55.129 25.358 19.241 1.00 25.09
     ATOM 1256 CG MET 325
     ATOM 1257 SD MET 325
                                53.714 26.409 19.672 1.00 27.29
     ATOM 1258 CE MET 325
                                52.503 25.220 20.084 1.00 20.67
     ATOM 1259 C MET 325
                               56.995 24.736 22.635 1.00 28.94
     ATOM 1260 O MET 325
                               56.881 23.510 22.672 1.00 32.94
     ATOM 1261 N SER 326
                               57.642 25.418 23.569 1.00 29.36
     ATOM 1262 CA SER 326
                               58.311 24.759 24.680 1.00 31.62
     ATOM 1263 CB SER 326
10
                                59.554 25.559 25.064 1.00 38.13
     ATOM 1264 OG SER 326
                                60.277 24.949 26.119 1.00 48.99
     ATOM 1265 C SER 326
                               57.361 24.653 25.871 1.00 33.69
     ATOM 1266 O SER 326
                               56.620 25.594 26.166 1.00 33.66
     ATOM 1267 N THR 327
                               57.356 23.499 26.536 1.00 38.27
     ATOM 1268 CA THR 327
                                56.497 23.306 27.701 1.00 38.98
15
     ATOM 1269 CB THR 327
                                55.875 21.896 27.730 1.00 33.30
     ATOM 1270 OG1 THR 327
                                56.908 20.911 27.627 1.00 44.01
     ATOM 1271 CG2 THR 327
                                54.888 21.722 26.587 1.00 38.09
                               57.239 23.570 29.018 1.00 42.88
     ATOM 1272 C THR 327
     ATOM 1273 O THR 327
                               56.702 23.325 30.099 1.00 43.36
20
     ATOM 1274 N ASP 328
                               58.462 24.091 28.924 1.00 45.92
     ATOM 1275 CA ASP 328
                               59.268 24.410 30.104 1.00 49.59
     ATOM 1276 CB ASP 328
                                60.760 24.411 29.760 1.00 59.87
                                61.273 23.040 29.387 1.00 75.73
     ATOM 1277 CG ASP 328
25
     ATOM 1278 OD1 ASP 328
                                62.008 22.939 28.382 1.00 85.81
     ATOM 1279 OD2 ASP 328
                                60.946 22.063 30.098 1.00 85.56
     ATOM 1280 C ASP 328
                               58.873 25.767 30.673 1.00 48.50
     ATOM 1281 O ASP 328
                               59.725 26.609 30.961 1.00 57.50
     ATOM 1282 N ARG 329
                               57.569 25.980 30.805 1.00 49.62
     ATOM 1283 CA ARG 329
                                57.032 27.222 31.340 1.00 50.52
30
     ATOM 1284 CB ARG 329
                                56.400 28.080 30.230 1.00 53.57
                                57.376 28.828 29.324 1.00 51.09
     ATOM 1285 CG ARG 329
                                57.897 27.951 28.204 1.00 49.73
     ATOM 1286 CD ARG 329
     ATOM 1287 NE ARG 329
                                58.692 28.699 27.233 1.00 47.44
     ATOM 1288 CZ ARG 329
                                60.005 28.569 27.080 1.00 54.28
35
     ATOM 1289 NH1 ARG 329
                                60.688 27.722 27.839 1.00 58.35
     ATOM 1290 NH2 ARG 329
                                 60.631 29.256 26.136 1.00 51.92
     ATOM 1291 C ARG 329
                               55.970 26.870 32.375 1.00 51.90
     ATOM 1292 O ARG 329
                               55.378 25.790 32.324 1.00 50.77
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     ATOM 1293 N SER 330
                               55.728 27.784 33.303 1.00 50.56
     ATOM 1294 CA SER 330
                               54.744 27.564 34.349 1.00 50.67
     ATOM 1295 CB SER 330
                               55.271 28.108 35.678 1.00 46.64
     ATOM 1296 C SER 330
                               53.404 28.213 34.004 1.00 47.63
                               53.371 29.309 33.440 1.00 48.02
     ATOM 1297 O SER 330
45
     ATOM 1298 N GLY 331
                               52.314 27.496 34.277 1.00 44.44
     ATOM 1299 CA GLY 331
                                50.977 28.023 34.044 1.00 38.77
     ATOM 1300 C GLY 331
                               50.236 27.710 32.756 1.00 41.74
     ATOM 1301 O GLY 331
ATOM 1302 N LEU 332
                               49.147 28.246 32.537 1.00 49.57
                               50.783 26.841 31.912 1.00 39.75
50
     ATOM 1303 CA LEU 332
                               50,123 26.502 30.651 1.00 37.55
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51.107 25.829 29.694 1.00 32.36
     ATOM 1304 CB LEU 332
     ATOM 1305 CG LEU 332
                                52.268 26.659 29.153 1.00 34.40
    ATOM 1306 CD1 LEU 332
                                53.207 25.749 28.379 1.00 30.22
                                51.742 27.786 28.277 1.00 23.33
    ATOM 1307 CD2 LEU 332
                               48.921 25.589 30.834 1.00 36.73
    ATOM 1308 C LEU 332
                               48.987 24.608 31.577 1.00 39.29
     ATOM 1309 O LEU 332
    ATOM 1310 N LEU 333
                               47.822 25.925 30.168 1.00 36.07
                               46.615 25.107 30.215 1.00 39.58
    ATOM 1311 CA LEU 333
    ATOM 1312 CB LEU 333
                               45.384 25.906 29.754 1.00 41.08
    ATOM 1313 CG LEU 333
                                44.601 26.883 30.644 1.00 47.59
10
    ATOM 1314 CD1 LEU 333
                                44.268 26.213 31.961 1.00 45.65
                                45.366 28.171 30.874 1.00 47.42
    ATOM 1315 CD2 LEU 333
                               46.791 23.911 29.278 1.00 40.00
    ATOM 1316 C LEU 333
    ATOM 1317 O LEU 333
                               46.690 22.754 29.689 1.00 44.77
    ATOM 1318 N CYA 334
                               47.102 24.213 28.022 1.00 37.70
15
                                47.265 23.209 26.968 1.00 36.04
     ATOM 1319 CA CYA 334
                                46.815 23.808 25.635 1.00 40.64
    ATOM 1320 CB CYA 334
                                45.280 24.738 25.758 1.00 44.31
    ATOM 1321 SG CYA 334
    ATOM 1322 AS CYA 334
                                43.972 22.946 25.380 1.00 76.30
20
    ATOM 1323 C CYA 334
                               48.668 22.617 26.815 1.00 34.91
    ATOM 1324 O CYA 334
                               49.237 22.615 25.722 1.00 37.63
    ATOM 1325 N VAL 335
                               49.189 22.056 27.903 1.00 35.43
                               50.518 21.452 27.909 1.00 34.27
    ATOM 1326 CA VAL 335
                                50.861 20.868 29.298 1.00 34.21
     ATOM 1327 CB VAL 335
                               52.261 20.258 29.292 1.00 33.66
     ATOM 1328 CG1 VAL 335
25
                                50.755 21.945 30.362 1.00 31.77
    ATOM 1329 CG2 VAL 335
                               50.662 20.349 26.865 1.00 37.14
    ATOM 1330 C VAL 335
     ATOM 1331 O VAL 335
                               51.639 20.320 26.114 1.00 37.59
     ATOM 1332 N ASP 336
                               49.683 19.451 26.813 1.00 39.99
    ATOM 1333 CA ASP 336
                                49.705 18.339 25.866 1.00 41.64
30
     ATOM 1334 CB ASP 336
                               48.532 17.392 26.146 1.00 54.27
                               48.596 16.118 25.322 1.00 67.42
    ATOM 1335 CG ASP 336
                               47.915 16.049 24.274 1.00 70.98
    ATOM 1336 OD1 ASP 336
     ATOM 1337 OD2 ASP 336
                              49.337 15.191 25.717 1.00 76.88
                              49.702 18.762 24.393 1.00 38.31
     ATOM 1338 C ASP 336
35
    ATOM 1339 O ASP 336
                               50.469 18.229 23.586 1.00 37.46
    ATOM 1340 N LYS 337
                               48.853 19.729 24.052 1.00 30.23
                               48.740 20.211 22.676 1.00 29.21
     ATOM 1341 CA LYS 337
                               47.561 21.189 22.559 1.00 30.53
    ATOM 1342 CB LYS 337
                                47.012 21.360 21.162 1.00 51.63
40
     ATOM 1343 CG LYS 337
                               45.636 21.997 21.186 1.00 59.57
     ATOM 1344 CD LYS 337
     ATOM 1345 CE LYS 337
                               45.066 22.115 19.774 1.00 66.05
                               43.673 22.693 19.776 1.00 67.20
     ATOM 1346 NZ LYS 337
     ATOM 1347 C LYS 337
                               50.054 20.873 22.249 1.00 28.33
                               50.581 20.594 21.170 1.00 26.08
     ATOM 1348 O LYS 337
45
     ATOM 1349 N ILE 338
                              50.609 21.696 23.141 1.00 26.74
                               51.873 22.390 22.902 1.00 25.42
     ATOM 1350 CA ILE 338
     ATOM 1351 CB ILE 338
                               52.177 23.379 24.052 1.00 23.57
     ATOM 1352 CG2 ILE 338
                               53.559 23.991 23.874 1.00 22.59
                               51.105 24.471 24.096 1.00 23.57
50
    ATOM 1353 CG1 ILE 338
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51.157 25.362 25.333 1.00 24.30
    ATOM 1354 CD1 ILE 338
                              53.018 21.382 22.768 1.00 29.20
    ATOM 1355 C ILE 338
    ATOM 1356 O ILE 338
                              53.905 21.537 21.916 1.00 31.59
                               52.977 20.340 23.595 1.00 34.82
    ATOM 1357 N GLU 339
                                53.980 19.277 23.597 1.00 34.23
    ATOM 1358 CA GLU 339
                                53.639 18.256 24.681 1.00 40.38
    ATOM 1359 CB GLU 339
                                54.785 17.354 25.072 1.00 54.98
    ATOM 1360 CG GLU 339
                                55.644 17.964 26.178 1.00 71.26
    ATOM 1361 CD GLU 339
    ATOM 1362 OE1 GLU 339
                                56.766 18.444 25.858 1.00 77.82
                                55.170 17.985 27.349 1.00 65.14
    ATOM 1363 OE2 GLU 339
10
                               53.972 18.582 22.231 1.00 34.42
    ATOM 1364 C GLU 339
                               55.018 18.431 21.590 1.00 29.41
    ATOM 1365 O GLU 339
    ATOM 1366 N LYS 340
                               52.778 18.189 21.786 1.00 34.13
                               52.592 17.513 20.502 1.00 32.05
    ATOM 1367 CA LYS 340
    ATOM 1368 CB LYS 340
                               51.121 17.105 20.325 1.00 34.59
15
                               53.064 18.390 19.337 1.00 32.56
    ATOM 1369 C LYS 340
    ATOM 1370 O LYS 340
                               53.762 17.913 18.441 1.00 32.93
                               52.725 19.677 19.374 1.00 31.42
    ATOM 1371 N SER 341
                              53.134 20.621 18.334 1.00 27.79
    ATOM 1372 CA SER 341
    ATOM 1373 CB SER 341
                               52.559 22.009 18.601 1.00 27.85
20
                               51.149 21.966 18.579 1.00 47.20
    ATOM 1374 OG SER 341
                               54.647 20.713 18.240 1.00 26.01
    ATOM 1375 C SER 341
                               55,205 20,706 17,139 1.00 27,10
    ATOM 1376 O SER 341
                               55.318 20.794 19.389 1.00 24.25
    ATOM 1377 N GLN 342
                                56.771 20.875 19.392 1.00 27.16
    ATOM 1378 CA GLN 342
25
                                57,309 21,089 20,799 1.00 25.60
    ATOM 1379 CB GLN 342
    ATOM 1380 CG GLN 342
                                58.768 21.466 20.777 1.00 27.99
    ATOM 1381 CD GLN 342
                                59.407 21.429 22.133 1.00 29.58
    ATOM 1382 OE1 GLN 342
                                60.123 22.356 22.513 1.00 31.18
                                59.184 20.345 22.868 1.00 29.17
    ATOM 1383 NE2 GLN 342
30
    ATOM 1384 C GLN 342
                               57.377 19.609 18.786 1.00 28.45
                               58.378 19.675 18.062 1.00 29.79
     ATOM 1385 O GLN 342
    ATOM 1386 N GLU 343
                               56.777 18.458 19.078 1.00 26.58
    ATOM 1387 CA GLU 343
                                57.251 17.190 18.525 1.00 30.07
     ATOM 1388 CB GLU 343
                                56.462 16.016 19.114 1.00 40.79
35
     ATOM 1389 CG GLU 343
                                56.812 15.700 20.568 1.00 61.22
    ATOM 1390 CD GLU 343
                                55.951 14.594 21.166 1.00 71.76
                                55.472 13.719 20.405 1.00 76.73
     ATOM 1391 OE1 GLU 343
                                55.758 14.601 22.403 1.00 74.09
     ATOM 1392 OE2 GLU 343
                               57.097 17.225 17.001 1.00 25.87
    ATOM 1393 C GLU 343
40
     ATOM 1394 O GLU 343
                               58.008 16.842 16.260 1.00 27.26
     ATOM 1395 N ALA 344
                               55.947 17.727 16.550 1.00 23.70
                                55.647 17.853 15.124 1.00 22.16
     ATOM 1396 CA ALA 344
                                54.275 18.489 14.927 1.00 21.18
     ATOM 1397 CB ALA 344
                               56.729 18.694 14.454 1.00 21.24
     ATOM 1398 C ALA 344
45
     ATOM 1399 O ALA 344
                               57.303 18.284 13.438 1.00 26.47
                               57.048 19.840 15.055 1.00 22.48
     ATOM 1400 N TYR 345
                                58.073 20.738 14.531 1.00 21.41
     ATOM 1401 CA TYR 345
     ATOM 1402 CB TYR 345
                                58.085 22.059 15.304 1.00 20.10
     ATOM 1403 CG TYR 345
                                57.023 23.015 14.830 1.00 15.87
50
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ATOM 1404 CD1 TYR 345
                                56.004 23.434 15.682 1.00 10.54
                                54.983 24.259 15.225 1.00 17.09
    ATOM 1405 CE1 TYR 345
                                57.003 23.448 13.505 1.00 16.86
    ATOM 1406 CD2 TYR 345
                                55.991 24.269 13.036 1.00 16.84
    ATOM 1407 CE2 TYR 345
                                54.984 24.668 13.896 1.00 17.97
    ATOM 1408 CZ TYR 345
                                53.963 25.455 13.406 1.00 27.11
    ATOM 1409 OH TYR 345
                               59.465 20.120 14.548 1.00 24.43
    ATOM 1410 C TYR 345
                               60.238 20.291 13.597 1.00 24.69
    ATOM 1411 O TYR 345
                               59.777 19.401 15.621 1.00 26.75
    ATOM 1412 N LEU 346
                                61.074 18.746 15.767 1.00 25.06
    ATOM 1413 CA LEU 346
10
                                61.207 18.108 17.150 1.00 24.59
    ATOM 1414 CB LEU 346
                                61.637 19.076 18.252 1.00 26.46
    ATOM 1415 CG LEU 346
                                61.387 18.468 19.610 1.00 26.46
    ATOM 1416 CD1 LEU 346
                                63.101 19.437 18.076 1.00 21.78
     ATOM 1417 CD2 LEU 346
                               61.322 17.713 14.683 1.00 23.24
     ATOM 1418 C LEU 346
15
                               62.416 17.645 14.127 1.00 27.54
     ATOM 1419 O LEU 346
                               60.314 16.900 14.395 1.00 25.75
     ATOM 1420 N LEU 347
                                60.437 15.881 13.356 1.00 25.41
     ATOM 1421 CA LEU 347
                                59.208 14.970 13.330 1.00 23.78
     ATOM 1422 CB LEU 347
                                59.302 13.713 14.190 1.00 31.85
     ATOM 1423 CG LEU 347
20
                                58.004 12.928 14.089 1.00 39.88
     ATOM 1424 CD1 LEU 347
                                60.483 12.864 13.738 1.00 27.65
     ATOM 1425 CD2 LEU 347
                               60.611 16.535 11.998 1.00 23.22
     ATOM 1426 C LEU 347
                               61.468 16.133 11.211 1.00 28.58
     ATOM 1427 O LEU 347
                               59.784 17.542 11.731 1.00 26.40
     ATOM 1428 N ALA 348
25
                                59.840 18.273 10.474 1.00 23.85
     ATOM 1429 CA ALA 348
                                58.732 19.324 10.433 1.00 25.27
     ATOM 1430 CB ALA 348
                               61.210 18.924 10.337 1.00 23.69
     ATOM 1431 C ALA 348
                                61.847 18.835 9.288 1.00 29.11
     ATOM 1432 O ALA 348
                               61.678 19.506 11.438 1.00 24.71
     ATOM 1433 N PHE 349
30
                                62.973 20.181 11.493 1.00 20.48
     ATOM 1434 CA PHE 349
                                63.164 20.772 12.900 1.00 17.84
     ATOM 1435 CB PHE 349
                                64.334 21.721 13.031 1.00 14.90
     ATOM 1436 CG PHE 349
                                65.109 22.069 11.933 1.00 17.58
     ATOM 1437 CD1 PHE 349
                                 64.651 22.269 14.271 1.00 24.77
     ATOM 1438 CD2 PHE 349
35
                                66.185 22.944 12.063 1.00 20.26
     ATOM 1439 CE1 PHE 349
                                65.727 23.147 14.413 1.00 23.83
     ATOM 1440 CE2 PHE 349
                                66.494 23.486 13.299 1.00 20.36
     ATOM 1441 CZ PHE 349
                               64.084 19.181 11.159 1.00 23.43
     ATOM 1442 C PHE 349
                                64.916 19.427 10.278 1.00 24.35
     ATOM 1443 O PHE 349
40
                                64.057 18.028 11.820 1.00 25.79
     ATOM 1444 N GLU 350
                                 65.060 16.991 11.606 1.00 26.75
     ATOM 1445 CA GLU 350
                                64.813 15.822 12.567 1.00 29.56
     ATOM 1446 CB GLU 350
                                 65.774 14.661 12.391 1.00 39.94
     ATOM 1447 CG GLU 350
                                 65.574 13.549 13.407 1.00 45.06
     ATOM 1448 CD GLU 350
45
                                 64.413 13.192 13.715 1.00 49.26
     ATOM 1449 OE1 GLU 350
                                 66.593 13.017 13.887 1.00 56.67
     ATOM 1450 OE2 GLU 350
                                65.051 16.494 10.162 1.00 26.95
     ATOM 1451 C GLU 350
                                66.096 16.398 9.513 1.00 28.77
     ATOM 1452 O GLU 350
                               63.858 16.219 9.652 1.00 22.56
     ATOM 1453 N HIS 351
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63.699 15.728 8.294 1.00 22.20
    ATOM 1454 CA HIS 351
                               62.263 15.265 8.083 1.00 22.47
    ATOM 1455 CB HIS 351
                               61.881 14.106 8.947 1.00 23.61
    ATOM 1456 CG HIS 351
                               62.633 13.300 9.739 1.00 27.65
    ATOM 1457 CD2 HIS 351
                                60.585 13.653 9.069 1.00 26.13
    ATOM 1458 ND1 HIS 351
                               60.548 12.629 9.898 1.00 22.87
    ATOM 1459 CE1 HIS 351
                               61.779 12.393 10.319 1.00 27.53
    ATOM 1460 NE2 HIS 351
                              64.135 16.764 7.259 1.00 21.76
    ATOM 1461 C HIS 351
                              64.708 16.419 6.226 1.00 27.02
    ATOM 1462 O HIS 351
                               63.909 18.041 7.555 1.00 18.26
    ATOM 1463 N TYR 352
10
                                64.327 19.101 6.649 1.00 16.94
    ATOM 1464 CA TYR 352
                                63.749 20.455 7.066 1.00 19.07
    ATOM 1465 CB TYR 352
                                64.107 21.534 6.081 1.00 21.11
    ATOM 1466 CG TYR 352
    ATOM 1467 CD1 TYR 352
                                63.518 21.564 4.819 1.00 21.33
                                63.921 22.482 3.859 1.00 21.06
    ATOM 1468 CE1 TYR 352
15
    ATOM 1469 CD2 TYR 352
                                65.105 22.462 6.367 1.00 22.07
                                65.515 23.388 5.412 1.00 25.40
    ATOM 1470 CE2 TYR 352
                                64.921 23.384 4.161 1.00 21.90
     ATOM 1471 CZ TYR 352
                                65.334 24.268 3.197 1.00 23.57
     ATOM 1472 OH TYR 352
                               65.853 19.156 6.657 1.00 18.49
     ATOM 1473 C TYR 352
20
     ATOM 1474 O TYR 352
                               66.487 19.323 5.609 1.00 24.99
                               66.451 19.008 7.836 1.00 24.64
     ATOM 1475 N VAL 353
     ATOM 1476 CA VAL 353
                                67.904 19.011 7.955 1.00 22.20
                                68.350 18.925 9.440 1.00 23.72
     ATOM 1477 CB VAL 353
                                 69.838 18.597 9.546 1.00 21.24
25
     ATOM 1478 CG1 VAL 353
                                 68.063 20.245 10.142 1.00 20.07
     ATOM 1479 CG2 VAL 353
                               68.452 17.829 7.146 1.00 25.07
     ATOM 1480 C VAL 353
     ATOM 1481 O VAL 353
ATOM 1482 N ASN 354
                               69,467 17.955 6.457 1.00 24.75
                               67.768 16.690 7.221 1.00 24.59
     ATOM 1483 CA ASN 354
                                68.171 15.502 6.474 1.00 25.64
30
                                67.223 14.331 6.751 1.00 26.05
     ATOM 1484 CB ASN 354
                                67.368 13.763 8.151 1.00 30.27
     ATOM 1485 CG ASN 354
                                 66.443 13.139 8.672 1.00 33.71
     ATOM 1486 OD1 ASN 354
                                 68.529 13.959 8.765 1.00 34.78
     ATOM 1487 ND2 ASN 354
                               68.143 15.813 4.981 1.00 30.50
     ATOM 1488 C ASN 354
35
                               69.042 15.423 4.233 1.00 33.73
     ATOM 1489 O ASN 354
                               67.098 16.519 4.555 1.00 30.54
     ATOM 1490 N HIS 355
                                66.926 16.901 3.157 1.00 26.02
     ATOM 1491 CA HIS 355
                                65.535 17.521 2.953 1.00 29.93
     ATOM 1492 CB HIS 355
                                65.367 18.217 1.638 1.00 37.91
     ATOM 1493 CG HIS 355
40
                                65.654 19.486 1.264 1.00 31.26
     ATOM 1494 CD2 HIS 355
                                64.861 17.593 0.518 1.00 32.67
     ATOM 1495 ND1 HIS 355
     ATOM 1496 CE1 HIS 355
                                64.843 18.447 -0.488 1.00 33.22
                                65.322 19.601 -0.061 1.00 32.69
     ATOM 1497 NE2 HIS 355
                               68.009 17.851 2.652 1.00 24.29
45
     ATOM 1498 C HIS 355
                               68.381 17.798 1.484 1.00 26.82
     ATOM 1499 O HIS 355
                                68.484 18.735 3.526 1.00 29.72
     ATOM 1500 N ARG 356
                                 69.516 19.711 3.167 1.00 26.65
     ATOM 1501 CA ARG 356
                                69.593 20.804 4.225 1.00 22.74
     ATOM 1502 CB ARG 356
                                68.409 21.735 4.222 1.00 21.64
     ATOM 1503 CG ARG 356
50
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68.757 23.024 3.524 1.00 28.04
    ATOM 1504 CD ARG 356
                                69.550 23.900 4.380 1.00 33.79
    ATOM 1505 NE ARG 356
    ATOM 1506 CZ ARG 356
                                70.508 24.716 3.952 1.00 29.26
                                70.814 24.776 2.667 1.00 29.08
    ATOM 1507 NH1 ARG 356
                                71.136 25.493 4.816 1.00 33.61
    ATOM 1508 NH2 ARG 356
                               70.904 19.115 2.950 1.00 27.58
    ATOM 1509 C ARG 356
                               71.757 19.740 2.312 1.00 31.44
    ATOM 1510 O ARG 356
                               71.140 17.937 3.519 1.00 30.56
    ATOM 1511 N LYS 357
    ATOM 1512 CA LYS 357
                               72.422 17.244 3.390 1.00 34.56
                               72.500 16.518 2.043 1.00 39.66
    ATOM 1513 CB LYS 357
10
                               71.476 15.402 1.871 1.00 42.16
    ATOM 1514 CG LYS 357
                               71.674 14.676 0.550 1.00 54.23
    ATOM 1515 CD LYS 357
                               70.691 13.523 0.371 1.00 61.97
    ATOM 1516 CE LYS 357
    ATOM 1517 NZ LYS 357
                               69.288 13.974 0.162 1.00 65.88
                               73.665 18.119 3.606 1.00 36.73
    ATOM 1518 C LYS 357
15
                               74.522 18.248 2.728 1.00 40.70
    ATOM 1519 O LYS 357
    ATOM 1520 N HIS 358
                              73.738 18.732 4.786 1.00 33.69
                               74.863 19.581 5.163 1.00 33.59
    ATOM 1521 CA HIS 358
                               74.660 20.155 6.571 1.00 32.07
    ATOM 1522 CB HIS 358
20
    ATOM 1523 CG HIS 358
                               73.593 21.200 6.666 1.00 29.74
                               72.245 21.098 6.736 1.00 23.35
    ATOM 1524 CD2 HIS 358
                                73.876 22.547 6.731 1.00 28.13
    ATOM 1525 ND1 HIS 358
                               72.752 23.231 6.834 1.00 26.94
    ATOM 1526 CE1 HIS 358
    ATOM 1527 NE2 HIS 358
                               71.747 22.373 6.838 1.00 23.32
                              76.121 18.720 5.180 1.00 37.98
    ATOM 1528 C HIS 358
25
                              76.087 17.581 5.654 1.00 41.07
    ATOM 1529 O HIS 358
                               77.231 19.261 4.690 1.00 44.20
    ATOM 1530 N ASN 359
    ATOM 1531 CA ASN 359
                                78.492 18.523 4.676 1.00 49.72
     ATOM 1532 CB ASN 359
                                79.406 19.053 3.572 1.00 46.66
    ATOM 1533 C ASN 359
                               79.174 18.648 6.039 1.00 51.77
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     ATOM 1534 O ASN 359
                               80.356 18.985 6.122 1.00 57.32
    ATOM 1535 N ILE 360
                              78.414 18.383 7.101 1.00 51.04
                               78.906 18.471 8.477 1.00 48.24
    ATOM 1536 CA ILE 360
                               78.340 19.721 9.207 1.00 47.20
    ATOM 1537 CB ILE 360
    ATOM 1538 CG2 ILE 360
                               78.781 19.741 10.673 1.00 43.50
35
    ATOM 1539 CG1 ILE 360
                               78.777 21.005 8.491 1.00 45.94
                               78.157 22.262 9.050 1.00 43.00
    ATOM 1540 CD1 ILE 360
                              78.462 17.222 9.239 1.00 47.23
     ATOM 1541 C ILE 360
                              77.272 16.901 9.278 1.00 45.13
     ATOM 1542 O ILE 360
                               79.416 16.490 9.838 1.00 48.61
     ATOM 1543 N PRO 361
40
                                80.869 16.705 9.729 1.00 50.93
     ATOM 1544 CD PRO 361
                                79.129 15.270 10.599 1.00 45.46
     ATOM 1545 CA PRO 361
                                80.524 14.725 10.927 1.00 49.01
     ATOM 1546 CB PRO 361
                                81.402 15.307 9.862 1.00 54.41
     ATOM 1547 CG PRO 361
                               78.330 15.514 11.879 1.00 36.54
     ATOM 1548 C PRO 361
45
                               78.666 16.394 12.672 1.00 39.83
     ATOM 1549 O PRO 361
                              77.282 14.716 12.075 1.00 31.35
     ATOM 1550 N HIS 362
                               76.430 14.798 13.264 1.00 33.34
     ATOM 1551 CA HIS 362
                               77.246 14.495 14.524 1.00 33.77
     ATOM 1552 CB HIS 362
                               78.129 13.292 14.397 1.00 34.40
50
    ATOM 1553 CG HIS 362
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77.837 11.999 14.130 1.00 32.60
     ATOM 1554 CD2 HIS 362
                                79.501 13.362 14.506 1.00 36.14
     ATOM 1555 ND1 HIS 362
                                80.017 12.160 14.311 1.00 36.26
     ATOM 1556 CE1 HIS 362
                                79.029 11.316 14.080 1.00 35.73
    ATOM 1557 NE2 HIS 362
                              75.778 16.164 13.389 1.00 33.55
     ATOM 1558 C HIS 362
                               75.539 16.652 14.495 1.00 31.93
     ATOM 1559 O HIS 362
                               75.449 16.748 12.240 1.00 35.83
     ATOM 1560 N PHE 363
                                74.834 18.067 12.166 1.00 30.93
     ATOM 1561 CA PHE 363
     ATOM 1562 CB PHE 363
                                74.464 18.394 10.712 1.00 28.82
                                73.959 19.797 10.514 1.00 26.59
    ATOM 1563 CG PHE 363
10
    ATOM 1564 CD1 PHE 363
                                74.846 20.843 10.301 1.00 26.96
     ATOM 1565 CD2 PHE 363
                                72.596 20.076 10.575 1.00 27.51
    ATOM 1566 CE1 PHE 363
                                74.384 22.151 10.155 1.00 31.83
                                72.124 21.378 10.433 1.00 26.65
     ATOM 1567 CE2 PHE 363
                                73.019 22.417 10.223 1.00 24.42
     ATOM 1568 CZ PHE 363
15
    ATOM 1569 C PHE 363
                               73.613 18.235 13.063 1.00 28.73
    ATOM 1570 O PHE 363
                               73.550 19.174 13.848 1.00 25.33
                               72.663 17.310 12.969 1.00 22.89
     ATOM 1571 N TRP 364
    ATOM 1572 CA TRP 364
                                71.443 17.405 13.760 1.00 24.19
                                70.481 16.254 13.439 1.00 26.31
     ATOM 1573 CB TRP 364
20
     ATOM 1574 CG TRP 364
                                69.198 16.275 14.228 1.00 20.24
                                68.213 17.325 14.262 1.00 24.50
     ATOM 1575 CD2 TRP 364
                                67.175 16.894 15.120 1.00 25.84
     ATOM 1576 CE2 TRP 364
                                68.106 18.583 13.652 1.00 25.83
     ATOM 1577 CE3 TRP 364
                                68.731 15.289 15.040 1.00 23.61
     ATOM 1578 CD1 TRP 364
25
     ATOM 1579 NE1 TRP 364
                                67.515 15.648 15.579 1.00 32.26
                                66.048 17.674 15.386 1.00 21.95
     ATOM 1580 CZ2 TRP 364
                                66.979 19.360 13.919 1.00 20.73
     ATOM 1581 CZ3 TRP 364
     ATOM 1582 CH2 TRP 364
                                 65.967 18.899 14.779 1.00 22.37
                               71.663 17.551 15.267 1.00 28.84
    ATOM 1583 C TRP 364
30
                               71.246 18.554 15.839 1.00 31.25
     ATOM 1584 O TRP 364
                               72.305 16.568 15.932 1.00 29.69
     ATOM 1585 N PRO 365
     ATOM 1586 CD PRO 365
                                72.790 15.245 15.497 1.00 30.89
     ATOM 1587 CA PRO 365
                                72.499 16.748 17.373 1.00 25.62
                                73.195 15.451 17.810 1.00 25.50
     ATOM 1588 CB PRO 365
35
                                73.804 14.915 16.560 1.00 34.15
     ATOM 1589 CG PRO 365
                               73.320 18.002 17.698 1.00 24.07
     ATOM 1590 C PRO 365
                               73.079 18.654 18.711 1.00 23.58
     ATOM 1591 O PRO 365
                               74.250 18.365 16.820 1.00 24.09
     ATOM 1592 N LYS 366
                                75.063 19.562 17.027 1.00 29.44
     ATOM 1593 CA LYS 366
40
     ATOM 1594 CB LYS 366
                                76.131 19.681 15.945 1.00 27.18
                                77.341 18.802 16.149 1.00 23.71
     ATOM 1595 CG LYS 366
     ATOM 1596 CD LYS 366
                                78.304 19.019 15.001 1.00 27.50
     ATOM 1597 CE LYS 366
                                79.624 18.329 15.231 1.00 35.88
                                80.550 18.591 14.097 1.00 41.92
45
     ATOM 1598 NZ LYS 366
                               74.195 20.820 17.012 1.00 32.76
     ATOM 1599 C LYS 366
                               74.326 21.694 17.873 1.00 36.13
     ATOM 1600 O LYS 366
                               73.307 20.907 16.028 1.00 33.70
     ATOM 1601 N LEU 367
     ATOM 1602 CA LEU 367
                                72.409 22.041 15.905 1.00 30.60
                                71.636 21.955 14.587 1.00 24.26
50
     ATOM 1603 CB LEU 367
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ATOM 1604 CG LEU 367
                                70.675 23.103 14.274 1.00 32.42
     ATOM 1605 CD1 LEU 367
                                71.394 24.440 14.404 1.00 24.78
           1606 CD2 LEU 367
                                70.098 22.924 12.878 1.00 28.84
     ATOM
                               71.450 22.015 17.087 1.00 31.90
           1607 C LEU 367
    ATOM
                               71.113 23.052 17.655 1.00 39.20
    ATOM 1608 O LEU 367
 5
                               71.051 20.812 17.485 1.00 33.86
           1609 N LEU 368
     ATOM
                                70.144 20.617 18.608 1.00 32.97
    ATOM 1610 CA LEU 368
                                69.866 19.123 18.759 1.00 34.22
    ATOM 1611 CB LEU 368
                                68.458 18.633 19.084 1.00 38.15
     ATOM 1612 CG LEU 368
                                67.400 19.449 18.345 1.00 27.75
    ATOM 1613 CD1 LEU 368
10
                                68.374 17.154 18.733 1.00 31.51
    ATOM 1614 CD2 LEU 368
                               70.793 21.181 19.875 1.00 35.29
    ATOM 1615 C LEU 368
                               70.128 21.806 20.703 1.00 36.16
     ATOM 1616 O LEU 368
     ATOM 1617 N MET 369
                               72.106 21.001 19.994 1.00 41.13
     ATOM 1618 CA MET 369
                                72.857 21.504 21.139 1.00 40.92
15
           1619 CB MET 369
                                74.283 20.955 21.115 1.00 43.32
     ATOM
                                74.383 19.497 21.545 1.00 50.01
           1620 CG MET 369
     ATOM
                                75.997 18.770 21.190 1.00 56.63
           1621 SD MET 369
     ATOM
                                77.032 19.596 22.409 1.00 62.26
           1622 CE MET 369
     ATOM
                               72.872 23.032 21.186 1.00 43.46
20
    ATOM 1623 C MET 369
                               73.137 23.619 22.233 1.00 47.51
     ATOM 1624 O MET 369
                               72.594 23.673 20.053 1.00 41.60
     ATOM 1625 N LYS 370
                                72.561 25.131 19.988 1.00 34.48
     ATOM 1626 CA LYS 370
     ATOM 1627 CB LYS 370
                                72.689 25.623 18.546 1.00 31.53
                                74.012 25.278 17.896 1.00 30.76
     ATOM 1628 CG LYS 370
25
                                75.168 25.774 18.731 1.00 32.16
     ATOM 1629 CD LYS 370
     ATOM 1630 CE LYS 370
                                76.488 25.388 18.116 1.00 31.08
     ATOM 1631 NZ LYS 370
                                77.604 25.822 18.993 1.00 51.52
     ATOM 1632 C LYS 370
                               71.269 25.652 20.606 1.00 36.35
     ATOM 1633 O LYS 370
                               71.197 26.806 21.032 1.00 39.02
30
     ATOM 1634 N VAL 371
                               70.248 24.804 20.652 1.00 34.33
     ATOM 1635 CA VAL 371
                                68.975 25.186 21.249 1.00 36.27
     ATOM 1636 CB VAL 371
                                67.885 24.097 21.046 1.00 36.15
     ATOM 1637 CG1 VAL 371
                                 66.600 24.487 21.758 1.00 32.69
                                 67.612 23.892 19.567 1.00 33.75
     ATOM 1638 CG2 VAL 371
35
     ATOM 1639 C VAL 371
                               69.196 25.423 22.745 1.00 41.55
     ATOM 1640 O VAL 371
                               68.638 26.367 23.316 1.00 40.82
     ATOM 1641 N THR 372
                               70.018 24.581 23.378 1.00 40.42
     ATOM 1642 CA THR 372
                                70.300 24.733 24.804 1.00 41.69
                                71.037 23.499 25.397 1.00 42.36
     ATOM 1643 CB THR 372
                                 72.125 23.133 24.548 1.00 53.57
     ATOM 1644 OG1 THR 372
     ATOM 1645 CG2 THR 372
                                 70.090 22.313 25.523 1.00 43.54
     ATOM 1646 C THR 372
                               71.090 26.021 25.048 1.00 38.75
                               70.858 26.714 26.042 1.00 37.51
     ATOM 1647 O THR 372
                               71.987 26.360 24.122 1.00 36.73
45
     ATOM 1648 N ASP 373
                                72.768 27.594 24.223 1.00 30.96
     ATOM 1649 CA ASP 373
                                73.741 27.732 23.047 1.00 31.26
     ATOM 1650 CB ASP 373
     ATOM 1651 CG ASP 373
                                74.865 26.707 23.085 1.00 35.85
                                75.523 26.508 22.042 1.00 36.73
     ATOM 1652 OD1 ASP 373
                                75.102 26.103 24.153 1.00 39.92
     ATOM 1653 OD2 ASP 373
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71.797 28.769 24.230 1.00 31.30
    ATOM 1654 C ASP 373
                               71.926 29.689 25.039 1.00 35.37
    ATOM 1655 O ASP 373
                               70.804 28.711 23.348 1.00 27.72
    ATOM 1656 N LEU 374
                                69.783 29.751 23.257 1.00 28.18
    ATOM 1657 CA LEU 374
                                68.881 29.521 22.042 1.00 28.41
    ATOM 1658 CB LEU 374
                                69.391 30.055 20.703 1.00 29.87
    ATOM 1659 CG LEU 374
                                68.533 29.520 19.563 1.00 25.44
    ATOM 1660 CD1 LEU 374
    ATOM 1661 CD2 LEU 374
                                69.385 31.581 20.728 1.00 23.74
                               68.946 29.786 24.527 1.00 28.61
    ATOM 1662 C LEU 374
                               68.516 30.859 24.968 1.00 29.51
    ATOM 1663 O LEU 374
10
                               68.690 28.615 25.105 1.00 32.32
    ATOM 1664 N ARG 375
    ATOM 1665 CA ARG 375
                                67.925 28.532 26.345 1.00 33.19
                                67.758 27.074 26.776 1.00 41.70
    ATOM 1666 CB ARG 375
    ATOM 1667 CG ARG 375
                                66.360 26.524 26.609 1.00 51.03
    ATOM 1668 CD ARG 375
                                65.979 26.416 25.153 1.00 60.16
15
                                64.648 25.840 24.987 1.00 74.28
    ATOM 1669 NE ARG 375
                                64.324 24.587 25.296 1.00 79.34
    ATOM 1670 CZ ARG 375
    ATOM 1671 NH1 ARG 375
                                 65.233 23.756 25.796 1.00 80.84
                                 63.084 24.157 25.092 1.00 77.44
    ATOM 1672 NH2 ARG 375
20
    ATOM 1673 C ARG 375
                               68.692 29.296 27.423 1.00 32.02
                               68.132 30.150 28.108 1.00 30.42
    ATOM 1674 O ARG 375
    ATOM 1675 N MET 376
                               69.993 29.020 27.521 1.00 32.30
    ATOM 1676 CA MET 376
                                70.860 29.668 28.499 1.00 36.82
                                72.278 29.097 28.433 1.00 45.36
    ATOM 1677 CB MET 376
                                72.375 27.645 28.866 1.00 66.71
    ATOM 1678 CG MET 376
25
                                74.078 27.057 28.966 1.00 89.64
    ATOM 1679 SD MET 376
    ATOM 1680 CE MET 376
                                74.256 26.229 27.400 1.00 85.51
    ATOM 1681 C MET 376
                               70.880 31.182 28.310 1.00 37.49
    ATOM 1682 O MET 376
                               70.780 31.928 29.281 1.00 39.99
    ATOM 1683 N ILE 377
                              71.008 31.630 27.060 1.00 33.14
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    ATOM 1684 CA ILE 377
                               71.009 33.057 26.740 1.00 25.98
    ATOM 1685 CB ILE 377
                               71.181 33.291 25.211 1.00 22.79
    ATOM 1686 CG2 ILE 377
                                70.838 34,727 24.834 1.00 25.29
    ATOM 1687 CG1 ILE 377
                                72.606 32.947 24.785 1.00 21.42
    ATOM 1688 CD1 ILE 377
                                72.816 32.971 23.282 1.00 19.37
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    ATOM 1689 C ILE 377
                              69.690 33.664 27.228 1.00 27.11
                              69.676 34.727 27.856 1.00 28.09
    ATOM 1690 O ILE 377
                               68.584 32.969 26.975 1.00 29.34
    ATOM 1691 N GLY 378
                                67.292 33.457 27.418 1.00 30.41
    ATOM 1692 CA GLY 378
                               67.233 33.532 28.934 1.00 36.85
    ATOM 1693 C GLY 378
40
                               66.672 34.481 29.489 1.00 36.44
    ATOM 1694 O GLY 378
    ATOM 1695 N ALA 379
                               67.837 32.547 29.603 1.00 37.98
                                67.869 32.483 31.066 1.00 36.44
    ATOM 1696 CA ALA 379
                                68.415 31.133 31.528 1.00 35.63
    ATOM 1697 CB ALA 379
                               68.712 33.613 31.642 1.00 34.14
45
    ATOM 1698 C ALA 379
                               68.259 34.343 32.523 1.00 35.15
    ATOM 1699 O ALA 379
    ATOM 1700 N CYA 380
                               69.941 33.747 31.144 1.00 36.66
                                70.860 34.795 31.587 1.00 37.27
     ATOM 1701 CA CYA 380
                                72.172 34.728 30.810 1.00 36.85
     ATOM 1702 CB CYA 380
                                73.201 33.338 31.250 1.00 52.80
50
     ATOM 1703 SG CYA 380
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	ATOM	1704 AS CYA 380 74.942 33.593 29.823 1.00 65.79
	ATOM	1705 C CYA 380 70.230 36.165 31.398 1.00 38.70
	ATOM	1706 O CYA 380 70.337 37.033 32.270 1.00 45.73
	ATOM	1707 N HIS 381 69.555 36.354 30.265 1.00 37.32
5	ATOM	1708 CA HIS 381 68.906 37.623 29.994 1.00 32.11
	ATOM	1709 CB HIS 381 68.377 37.687 28.565 1.00 25.76
	ATOM	1710 CG HIS 381 67.596 38.932 28.285 1.00 20.30
	ATOM	1711 CD2 HIS 381 67.998 40.200 28.044 1.00 16.31
	ATOM	1712 ND1 HIS 381 66.218 38.971 28.336 1.00 22.06
10	ATOM	1713 CE1 HIS 381 65.807 40.210 28.146 1.00 21.20
	ATOM	1714 NE2 HIS 381 66.869 40.976 27.968 1.00 22.58
	ATOM	1715 C HIS 381 67.773 37.893 30.980 1.00 32.68
	ATOM	1716 O HIS 381 67.602 39.024 31.431 1.00 33.38
	ATOM	1717 N ALA 382 66.982 36.873 31.296 1.00 31.27
15	ATOM	1718 CA ALA 382 65.884 37.045 32.243 1.00 29.39
	ATOM	1719 CB ALA 382 65.121 35.742 32.409 1.00 25.18
	ATOM	1720 C ALA 382 66.420 37.531 33.596 1.00 34.32
	ATOM	1721 O ALA 382 65.902 38.501 34.160 1.00 37.79
	ATOM	1722 N SER 383 67.483 36.893 34.085 1.00 36.88
20	ATOM	1723 CA SER 383 68.100 37.268 35.361 1.00 39.74
	ATOM	1724 CB SER 383 69.233 36.297 35.719 1.00 42.58
	ATOM	1725 OG SER 383 68.734 35.010 36.049 1.00 61.85
	ATOM	1726 C SER 383 68.638 38.697 35.311 1.00 36.49
	ATOM	1727 O SER 383 68.443 39.480 36.243 1.00 43.81
25	ATOM	1728 N ARG 384 69.305 39.036 34.213 1.00 33.66
	ATOM	1729 CA ARG 384 69.866 40.367 34.043 1.00 35.39
	ATOM	1730 CB ARG 384 70.800 40.404 32.835 1.00 29.29 1731 CG ARG 384 71.590 41.679 32.731 1.00 29.20
	ATOM	1,51 00 1110 101
20	ATOM	1732 CD ARG 384 72.881 41.435 31.995 1.00 37.73 1733 NE ARG 384 73.657 42.663 31.850 1.00 48.97
30	ATOM	1755 112 1116 501 121651 1216
	ATOM	
	ATOM	
	ATOM	
25	ATOM	1737 C ARG 384 68.777 41.431 33.916 1.00 39.45 1738 O ARG 384 68.913 42.537 34.444 1.00 44.47
35	ATOM ATOM	1739 N PHE 385 67.673 41.077 33.270 1.00 36.42
	ATOM	1740 CA PHE 385 66.568 42.007 33.270 1.00 34.68
	ATOM	1741 CB PHE 385 65.444 41.393 32.262 1.00 30.21
	ATOM	1742 CG PHE 385 64.263 42.304 32.081 1.00 29.48
40	ATOM	1743 CD1 PHE 385 64.289 43.313 31.127 1.00 29.70
70	ATOM	1744 CD2 PHE 385 63.130 42.161 32.873 1.00 28.04
	ATOM	1745 CE1 PHE 385 63.203 44.169 30.966 1.00 33.50
	ATOM	1746 CE2 PHE 385 62.040 43.012 32.718 1.00 31.35
	ATOM	1747 CZ PHE 385 62.077 44.017 31.763 1.00 32.08
45	ATOM	1748 C PHE 385 66.040 42.412 34.468 1.00 35.76
, ,	ATOM	1749 O PHE 385 65.761 43.590 34.693 1.00 40.58
	ATOM	1750 N LEU 386 65.906 41.441 35.373 1.00 37.55
	ATOM	1751 CA LEU 386 65.429 41.706 36.735 1.00 41.01
	ATOM	1752 CB LEU 386 65.394 40.413 37.563 1.00 42.30
50	ATOM	1753 CG LEU 386 64.240 39.434 37.317 1.00 43.34

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64.559 38.066 37.912 1.00 43.50
    ATOM 1754 CD1 LEU 386
                                62.946 39.992 37.899 1.00 44.01
    ATOM 1755 CD2 LEU 386
                               66.342 42.735 37.405 1.00 40.08
    ATOM 1756 C LEU 386
                               65.875 43.632 38.112 1.00 42.08
    ATOM 1757 O LEU 386
                              67.643 42.613 37.153 1.00 34.86
    ATOM 1758 N HIS 387
                               68.631 43.537 37.700 1.00 39.09
    ATOM 1759 CA HIS 387
                               70.046 43.034 37.421 1.00 39.99
    ATOM 1760 CB HIS 387
                               70.402 41.791 38.172 1.00 56.37
    ATOM 1761 CG HIS 387
                               71.384 40.881 37.974 1.00 60.11
    ATOM 1762 CD2 HIS 387
                                69.711 41.370 39.290 1.00 60.40
    ATOM 1763 ND1 HIS 387
10
                               70.252 40.255 39.746 1.00 61.89
    ATOM 1764 CE1 HIS 387
    ATOM 1765 NE2 HIS 387
                               71.269 39.937 38.966 1.00 63.96
                              68.446 44.928 37.101 1.00 41.00
    ATOM 1766 C HIS 387
                              68.492 45.927 37.817 1.00 46.99
    ATOM 1767 O HIS 387
                               68.213 44.982 35.792 1.00 39.15
    ATOM 1768 N MET 388
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    ATOM 1769 CA MET 388
                                68.011 46.243 35.088 1.00 35.32
                                67.676 45.992 33.612 1.00 35.12
    ATOM 1770 CB MET 388
                                68.810 45.442 32.753 1.00 37.24
    ATOM 1771 CG MET 388
    ATOM 1772 SD MET 388
                                68.259 45.150 31.051 1.00 41.75
    ATOM 1773 CE MET 388
                                69.274 43.748 30.573 1.00 35.23
20
                               66.880 47.048 35.733 1.00 36.52
    ATOM 1774 C MET 388
                               66.994 48.265 35.888 1.00 43.39
    ATOM 1775 O MET 388
                               65.792 46.371 36.103 1.00 38.05
    ATOM 1776 N LYS 389
                                64.637 47.025 36.729 1.00 42.88
    ATOM 1777 CA LYS 389
                                63.481 46.035 36.866 1.00 47.83
25
    ATOM 1778 CB LYS 389
                                62.835 45.627 35.560 1.00 52.36
    ATOM 1779 CG LYS 389
    ATOM 1780 CD LYS 389
                                62.040 44.340 35.731 1.00 61.84
    ATOM 1781 CE LYS 389
                                60.978 44.451 36.814 1.00 69.04
                                60.254 43.162 36.987 1.00 70.00
    ATOM 1782 NZ LYS 389
                               64,983 47.587 38.107 1.00 43.99
    ATOM 1783 C LYS 389
30
                               64.455 48.621 38.525 1.00 44.22
    ATOM 1784 O LYS 389
                               65.851 46.878 38.816 1.00 45.50
    ATOM 1785 N VAL 390
                                66.290 47.286 40.142 1.00 47.76
    ATOM 1786 CA VAL 390
                                67.152 46.186 40.804 1.00 46.30
    ATOM 1787 CB VAL 390
    ATOM 1788 CG1 VAL 390
                                67.796 46.706 42.079 1.00 49.20
35
    ATOM 1789 CG2 VAL 390
                                66,305 44.962 41.097 1.00 42.69
     ATOM 1790 C VAL 390
                               67.109 48.571 40.070 1.00 47.25
                               66.811 49.540 40.760 1.00 48.67
     ATOM 1791 O VAL 390
                               68.115 48.580 39.199 1.00 44.11
     ATOM 1792 N GLU 391
                                69.009 49.721 39.047 1.00 45.79
     ATOM 1793 CA GLU 391
40
     ATOM 1794 CB GLU 391
                                70.266 49.311 38.273 1.00 45.78
    ATOM 1795 CG GLU 391
                                70,998 48.091 38.830 1.00 57.29
     ATOM 1796 CD GLU 391
                                71.479 48.268 40.261 1.00 61.20
     ATOM 1797 OE1 GLU 391
                                71.845 49.400 40.646 1.00 57.29
     ATOM 1798 OE2 GLU 391
                                71.496 47.263 41.001 1.00 63.69
45
                               68.410 50.959 38.391 1.00 49.16
     ATOM 1799 C GLU 391
     ATOM 1800 O GLU 391
                               68.463 52.055 38.956 1.00 58.82
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     ATOM 1898 CB VAL 404
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	ATOM	1907 CD1 PHE 405	62.283 41.625 27.672 1.00 33.90
5	ATOM	1908 CD2 PHE 405	62.157 39.281 28.138 1.00 31.62
	ATOM	1909 CE1 PHE 405	62.786 41.351 26.399 1.00 39.16
	ATOM	1910 CE2 PHE 405	62.657 38.997 26.872 1.00 33.33
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	ATOM	2 O1 HOH 502	69.618 40.719 13.009 1.00 23.00
	ATOM	3 O1 HOH 503	64.885 40.168 12.340 1.00 23.00
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	ATOM	6 O1 HOH 506	61.299 15.617 -0.595 1.00 23.00
	ATOM	7 O1 HOH 507	67.359 15.375 0.551 1.00 23.00
	ATOM	8 O1 HOH 508	67.230 12.002 -0.634 1.00 23.00
	ATOM	9 O1 HOH 509	66.906 12.467 3.855 1.00 23.00
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	ATOM	19 O1 HOH 519	50.338 23.299 7.662 1.00 41.19
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	ATOM	28 O1 HOH 528	67.871 36.399 6.419 1.00 66.52
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	ATOM	36 O1 HOH 536	58.575 52.330 31.881 1.00 23.00
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	ATOM	38 O1 HOH 538	61.736 40.280 35.059 1.00 60.53
	ATOM	39 O1 HOH 539	63.271 38.155 34.156 1.00 52.21
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	ATOM	48 O1 HOH	548	
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	ATOM	54 O1 HOH	554	69.504 11.968 14.083 1.00 23.00
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25	ATOM	65 O1 HOH	565	76.525 41.395 10.460 1.00 23.00
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	ATOM	72 O1 HOH	572	
	ATOM	73 O1 HOH	573	
25	ATOM	74 O1 HOH	574	
35	ATOM	75 O1 HOH	575	. 0.0
	ATOM	76 O1 HOH	576	
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40	ATOM	79 O1 HOH	579	76.954 22.077 18.425 1.00 46.50
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	ATOM	82 O1 HOH	582	83.586 42.305 18.576 1.00 23.00
	ATOM	83 O1 HOH	583	83.481 45.262 19.526 1.00 23.00
	ATOM	84 O1 HOH	584	66.787 32.864 33.796 1.00 23.00
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	ATOM	88 O1 HOH	588	52.774 25.054 32.650 1.00 57.81
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50	ATOM	90 O1 HOH	590	47.195 30.205 30.414 1.00 23.00

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     ATOM 2325 O1 IBR
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     END
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PCT/US98/25296 WO 99/26966

APPENDIX 6

TR_T3.PDB

REMARK rTR_t3 full length numbering

REMARK

5 REMARK Rfactor 0.221 Rfree 0.240

REMARK Resolution 5. 2.0 all reflections

REMARK conformation of MET 388 confirmed by SA_omit map

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392 10

REMARK cacodylate modeled as single arsenic atom

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

15 REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

20 REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

M.B. MURRAY, N.D.ZILZ, AUTH **JRNL**

25 N.L.MCCREARY, M.J.MACDONALD

> JRNL **AUTH 2 H.C.TOWLE**

TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA **JRNL**

CLONES FOR TWO

TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL

30 JRNL REF JBC V. 263 25 1988

> AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS JRNL

IDENTIFICATION OF A NOVEL THYROID HORMONE JRNL TITL RECEPTOR EXPRESSED

TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM **JRNL**

35 JRNL REF SCIENCE

V. 237 1987 AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM **JRNL**

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY ALTERNATIVE

TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR **JRNL**

GENE TRANSCRIPT 40

> REF NUC. ACIDS. RES. V. 16 12 1988 JRNL

REMARK

68.406 10.620 7.027 1.00 41.66 1 CB ARG 157 ATOM

69.926 10.540 6.997 1.00 44.48 2 CG ARG 157 ATOM 70.552 11.261 8.173 1.00 47.02

45 ATOM 3 CD ARG 157 70.112 10.680 9.435 1.00 49.73 ATOM 4 NE ARG 157

ATOM 5 CZ ARG 157 70.917 10.392 10.450 1.00 51.21

72.223 10.629 10.361 1.00 51.79 **ATOM** 6 NH1 ARG 157

```
ATOM
              7 NH2 ARG 157
                                70.405 9.871 11.556 1.00 51.92
     ATOM
              8 C ARG 157
                              66.308 9.993 5.774 1.00 36.48
              9 O ARG 157
                              66.047 10.318 4.622 1.00 38.84
     ATOM
     ATOM
             10 N ARG 157
                               68.479 9.473 4.839 1.00 41.22
                                67.734 9.580 6.135 1.00 39.98
     ATOM
             11 CA ARG 157
                               65.366 9.953 6.728 1.00 33.85
     ATOM
             12 N PRO 158
                               65.494 9.553 8.139 1.00 34.72
     ATOM
             13 CD PRO 158
             14 CA PRO 158
                               63.981 10.336 6.407 1.00 31.89
     ATOM
             15 CB PRO 158
                               63.219 10.015 7.694 1.00 31.87
     ATOM
                               64.260 10.158 8.759 1.00 33.55
             16 CG PRO 158
10
     ATOM
             17 C PRO 158
                              63.758 11.783 5.947 1.00 29.77
     ATOM
                               64.221 12.739 6.575 1.00 27.93
             18 O PRO 158
     ATOM
     ATOM
             19 N GLU 159
                               63.071 11.918 4.819 1.00 26.20
     ATOM
             20 CA GLU 159
                               62.759 13.217 4.239 1.00 24.07
15
     ATOM
             21 CB GLU 159
                               62.565 13.080 2.721 1.00 22.90
             22 CG GLU 159
                               63.847 12.933 1.916 1.00 22.04
     ATOM
     ATOM
             23 CD GLU 159
                               64.386 14.260 1.427 1.00 22.07
     ATOM
             24 OE1 GLU 159
                                63.577 15.175 1.203 1.00 24.63
     ATOM
             25 OE2 GLU 159
                                65.612 14.389 1.240 1.00 23.54
20
     ATOM
             26 C GLU 159
                               61.463 13.717 4.855 1.00 21.56
                               60.747 12.958 5.516 1.00 21.03
     ATOM
             27 O GLU 159
             28 N PRO 160
                              61.176 15.022 4.713 1.00 19.69
     ATOM
                               61.997 16.139 4.207 1.00 16.57
     ATOM
             29 CD PRO 160
             30 CA PRO 160
     ATOM
                               59.923 15.500 5.292 1.00 18.12
25
     ATOM
             31 CB PRO 160
                               59.935 16.990 4.955 1.00 15.65
     ATOM
             32 CG PRO 160
                               61.390 17.328 4.905 1.00 14.83
     ATOM
             33 C PRO 160
                              58.741 14.782 4.626 1.00 19.79
    ATOM
             34 O PRO 160
                              58.793 14.431 3.445 1.00 20.20
     ATOM
             35 N THR 161
                               57.713 14.497 5.412 1.00 20.15
30
     ATOM
             36 CA THR 161
                               56.525 13.846 4.901 1.00 20.73
     ATOM
             37 CB THR 161
                               55.672 13.274 6.060 1.00 20.77
    ATOM
             38 OG1 THR 161
                                55.195 14.348 6.881 1.00 21.74
     ATOM
             39 CG2 THR 161
                                56.489 12.324 6.917 1.00 19.52
     ATOM
             40 C THR 161
                              55.724 14.954 4.219 1.00 21.64
35
     ATOM
             41 O THR 161
                               56.010 16.139 4.421 1.00 23.13
             42 N PRO 162
                              54.701 14.596 3.425 1.00 21.21
     ATOM
             43 CD PRO 162
                               54.309 13.235 3.012 1.00 19.57
    ATOM
             44 CA PRO 162
                               53.884 15.602 2.751 1.00 21.01
    ATOM
     ATOM
             45 CB PRO 162
                               52.722 14.776 2.223 1.00 19.74
40
             46 CG PRO 162
                               53.387 13.490 1.861 1.00 20.34
     ATOM
    ATOM
             47 C PRO 162
                              53.391 16.643 3.753 1.00 22.52
             48 O PRO 162
                              53.508 17.851 3.526 1.00 21.68
    ATOM
             49 N GLU 163
                               52.880 16.151 4.878 1.00 23.01
    ATOM
             50 CA GLU 163
                               52.349 16.996 5.941 1.00 25.97
    ATOM
                               51.672 16.148 7.022 1.00 29.50
45
    ATOM
             51 CB GLU 163
                               50.476 15.312 6.543 1.00 37.07
    ATOM
             52 CG GLU 163
             53 CD GLU 163
                               50.865 14.159 5.614 1.00 41.36
    ATOM
             54 OE1 GLU 163
                                51.937 13.544 5.828 1.00 40.11
    ATOM
             55 OE2 GLU 163
                                50.094 13.874 4.660 1.00 46.16
     ATOM
50
     ATOM
             56 C GLU 163
                              53.415 17.879 6.581 1.00 24.92
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	A TO 1 4	57 O GLU 163	53.110 18.971 7.061 1.00 25.82
	ATOM	57 O GLU 163 58 N GLU 164	54.661 17.412 6.600 1.00 22.87
	ATOM ATOM	59 CA GLU 164	55.724 18.209 7.187 1.00 21.46
	ATOM	60 CB GLU 164	56.880 17.340 7.664 1.00 21.40
5	ATOM	61 CG GLU 164	56.509 16.508 8.886 1.00 20.30
ر	ATOM	62 CD GLU 164	57.557 15.483 9.243 1.00 20.07
	ATOM	63 OE1 GLU 164	58.409 15.186 8.385 1.00 19.80
	ATOM	64 OE2 GLU 164	57.532 14.977 10.385 1.00 21.00
	ATOM	65 C GLU 164	56.195 19.289 6.235 1.00 22.45
10	ATOM	66 O GLU 164	56.607 20.354 6.684 1.00 23.36
10	ATOM	67 N TRP 165	56.140 19.024 4.928 1.00 21.06
	ATOM	68 CA TRP 165	56.518 20.031 3.936 1.00 19.57
	ATOM	69 CB TRP 165	56.486 19.466 2.518 1.00 16.06
	ATOM	70 CG TRP 165	57.775 18.839 2.120 1.00 14.01
15	ATOM	71 CD2 TRP 165	59.055 19.480 2.037 1.00 13.26
13	ATOM	72 CE2 TRP 165	59.976 18.515 1.588 1.00 12.91
	ATOM	73 CE3 TRP 165	59.507 20.779 2.300 1.00 14.44
	ATOM	74 CD1 TRP 165	57.972 17.544 1.738 1.00 12.89
	ATOM	75 NEI TRP 165	59.290 17.343 1.413 1.00 12.80
20	ATOM	76 CZ2 TRP 165	61.328 18.805 1.388 1.00 15.06
	ATOM	77 CZ3 TRP 165	60.850 21.069 2.103 1.00 14.72
	ATOM	78 CH2 TRP 165	61.747 20.084 1.649 1.00 16.82
	ATOM	79 C TRP 165	55.553 21.210 4.056 1.00 18.93
	ATOM	80 O TRP 165	55.960 22.359 3.926 1.00 21.12
25	ATOM	81 N ASP 166	54.279 20.922 4.307 1.00 19.33
-	ATOM	82 CA ASP 166	53.262 21.963 4.483 1.00 20.35
	ATOM	83 CB ASP 166	51.864 21.353 4.672 1.00 20.22
	ATOM	84 CG ASP 166	51.302 20.748 3.386 1.00 23.36
	ATOM	85 OD1 ASP 166	51.746 21.153 2.296 1.00 23.42
30	ATOM	86 OD2 ASP 166	50.414 19.878 3.462 1.00 21.02
	ATOM	87 C ASP 166	53.623 22.785 5.712 1.00 21.02
	ATOM	88 O ASP 166	53.627 24.013 5.654 1.00 22.56
	ATOM	89 N LEU 167	53.926 22.096 6.813 1.00 20.50
	ATOM	90 CA LEU 167	54.312 22.726 8.071 1.00 21.37
35	ATOM	91 CB LEU 167	54.661 21.657 9.109 1.00 23.49
	ATOM	92 CG LEU 167	54.223 21.846 10.565 1.00 27.19
	ATOM	93 CD1 LEU 167	55.312 21.291 11.453 1.00 27.70
	ATOM	94 CD2 LEU 167	53.940 23.314 10.906 1.00 27.71
	ATOM	95 C LEU 167	55.541 23.602 7.839 1.00 20.72
40	ATOM	96 O LEU 167	55.601 24.748 8.294 1.00 22.98
	ATOM	97 N ILE 168	56.505 23.051 7.114 1.00 18.54
	ATOM	98 CA ILE 168	57.747 23.725 6.778 1.00 18.60
	ATOM	99 CB ILE 168	58.671 22.771 5.995 1.00 17.54
	ATOM	100 CG2 ILE 168	59.695 23.533 5.163 1.00 17.65
45	ATOM	101 CG1 ILE 168	59.330 21.794 6.972 1.00 20.27
	ATOM	102 CD1 ILE 168	60.048 20.631 6.322 1.00 17.96
	ATOM	103 C ILE 168	57.486 25.002 5.979 1.00 21.96
	ATOM	104 O ILE 168	58.045 26.064 6.291 1.00 23.06
5 .0	ATOM	105 N HIS 169	56.591 24.925 4.996 1.00 22.04
50	ATOM	106 CA HIS 169	56.285 26.092 4.164 1.00 21.21

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ATOM 108 CG HIS 169 ATOM 109 CD2 HIS 169 ATOM 110 ND1 HIS 169 ATOM 111 ND1 HIS 169 ATOM 111 CE1 HIS 169 ATOM 112 NE2 HIS 169 ATOM 112 NE2 HIS 169 ATOM 113 C HIS 169 ATOM 114 O HIS 169 ATOM 115 N VAL 170 ATOM 116 CA VAL 170 ATOM 117 CB VAL 170 ATOM 119 CG2 VAL 170 ATOM 119 CG2 VAL 170 ATOM 120 C VAL 170 ATOM 121 O VAL 170 ATOM 122 N ALA 171 ATOM 124 CB ALA 171 ATOM 125 C ALA 171 ATOM 126 O ALA 171 ATOM 127 N THR 172 ATOM 129 CB THR 172 ATOM 130 OG1 THR 172 ATOM 131 CG2 THR 172 ATOM 131 CG2 THR 172 ATOM 132 C THR 172 ATOM 133 O THR 172 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 CG1 U 173 ATOM 130 CG1 U 173 ATOM 131 CG2 THR 172 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 CG1 U 173 ATOM 130 CG1 U 173 ATOM 130 CG1 U 173 ATOM 131 CG2 THR 172 ATOM 132 C THR 172 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 CG1 U 173 ATOM 130 CG1 U 173 ATOM 131 CG2 U 173 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 CG1 U 173 ATOM 130 CG1 U 173 ATOM 130 CG1 U 173 ATOM 130 CG1 U 173 ATOM 131 CG2 U 173 ATOM 131 CG2 U 173 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 CG1 GLU 173 ATOM 130 CG1 U 17		ATOM	107 CB HIS 169	55.413 25.702 2.969 1.00 20.12
ATOM 109 CD2 HIS 169				
ATOM 110 ND1 HIS 169 55.457 23.764 1.357 1.00 17.90 ATOM 111 CEI HIS 169 56.327 23.096 0.625 1.00 20.10 ATOM 113 C HIS 169 55.615 27.198 4.959 1.00 20.61 ATOM 114 O HIS 169 55.615 27.198 4.959 1.00 20.61 ATOM 115 N VAL 170 54.632 26.821 5.769 1.00 20.01 ATOM 117 CB VAL 170 54.632 26.821 5.769 1.00 20.02 20.01 ATOM 119 CG2 VAL 170 54.926 29.12 27.785 6.580 1.00 20.52 ATOM 120 C VAL 170 54.891 28.241 1.00 22.32 ATOM 120 C VAL 170 54.891 28.234 9.182 1.00 1.00 ATOM				
5 ATOM 111 CE1 HIS 169 56.327 23.096 0.625 1.00 18.43 ATOM 112 NEZ HIS 169 57.513 23.660 0.772 1.00 20.10 ATOM 114 O HIS 169 55.615 27.198 4.959 1.00 20.01 ATOM 115 N VAL 170 55.615 27.198 4.959 1.00 20.08 ATOM 116 CA VAL 170 54.632 26.21 5.769 1.00 20.08 ATOM 117 CB VAL 170 54.632 26.21 5.769 1.00 20.02 ATOM 119 CG2 VAL 170 54.632 26.221 5.769 1.00 20.32 ATOM 119 CG2 VAL 170 52.224 28.113 8.366 1.00 20.23 ATOM 120 C VAL 170 54.891 28.477 7.521 1.00 20.58 ATOM 124 CB ALA 171 56.692 28.234 9.182				
ATOM 112 NE2 HIS 169 57.513 23.660 0.772 1.00 20.10 ATOM 113 C HIS 169 55.615 27.198 4.959 1.00 20.61 ATOM 115 N VAL 170 54.632 26.821 5.769 1.00 20.01	5			
ATOM 114 O HIS 169 55.615 27.198 4.959 1.00 20.61 ATOM 114 O HIS 169 55.979 28.370 4.836 1.00 20.08 ATOM 115 N VAL 170 54.632 26.821 5.769 1.00 20.01 10 ATOM 116 CA VAL 170 53.922 27.785 6.580 1.00 20.52 ATOM 117 CB VAL 170 52.816 27.120 7.384 1.00 21.33 ATOM 119 CG2 VAL 170 ATOM 119 CG2 VAL 170 54.891 28.477 7.521 1.00 20.58 ATOM 120 C VAL 170 54.926 29.704 7.554 1.00 22.32 ATOM 123 CA ALA 171 55.712 27.696 8.230 1.00 18.83 ATOM 123 CA ALA 171 56.692 28.234 9.182 1.00 18.34 ATOM 125 C ALA 171 57.335 29.151 8.533 1.00 17.84 ATOM 126 O ALA 171 58.084 30.200 9.091 1.00 18.67 ATOM 127 N THR 172 58.231 28.756 7.367 1.00 17.81 ATOM 129 CB THR 172 ATOM 130 OG1 THR 172 ATOM 131 CG2 THR 172 ATOM 133 O THR 172 ATOM 133 O THR 172 59.215 29.551 6.639 1.00 12.38 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 OE1 GLU 173 ATOM 130 OG1 THR 172 58.651 30.932 6.251 1.00 19.42 ATOM 130 OG1 THR 172 58.651 30.932 6.251 1.00 19.42 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 134 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.482 33.244 4.005 1.00 34.96 ATOM 147 CA ALA 174 55.483 33.29 9.20 1.00 18.80 ATOM 144 CA ALA 174 55.843 33.294 9.00 1.00 17.65 ATOM 148 N HIS 175 59.498 33.831 9.029 1.00 16.39 ATOM 148 N HIS 175 59.498 33.831 9.029 1.00 16.39 ATOM 148 N HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 150 CB HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
ATOM 115 N VAL 170		ATOM		55.615 27.198 4.959 1.00 20.61
ATOM		ATOM	114 O HIS 169	55.979 28.370 4.836 1.00 20.08
ATOM 117 CB VAL 170		ATOM	115 N VAL 170	54.632 26.821 5.769 1.00 20.01
ATOM 118 CG1 VAL 170	10	ATOM	116 CA VAL 170	53.922 27.785 6.580 1.00 20.52
ATOM 119 CG2 VAL 170 ATOM 120 C VAL 170 ATOM 121 O VAL 170 ATOM 121 O VAL 170 ATOM 122 N ALA 171 ATOM 123 CA ALA 171 ATOM 124 CB ALA 171 ATOM 125 C ALA 171 ATOM 126 O ALA 171 ATOM 127 N THR 172 ATOM 129 CB THR 172 ATOM 130 OG1 THR 172 ATOM 131 CG2 THR 172 ATOM 132 C THR 172 ATOM 133 O THR 172 ATOM 134 N GLU 173 ATOM 135 CA GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 OE1 GLU 173 ATOM 130 CGLU 173 ATOM 130 CGLU 173 ATOM 130 CG LU 173 ATOM 131 CG2 GLU 173 ATOM 136 CB GLU 173 ATOM 137 CG GLU 173 ATOM 138 CD GLU 173 ATOM 139 OE1 GLU 173 ATOM 140 OE2 GLU 173 ATOM 140 OE2 GLU 173 ATOM 141 C GLU 173 ATOM 142 O GLU 173 ATOM 144 CA ALA 174 ATOM 145 CB ALA 174 ATOM 146 C ALA 174 ATOM 147 O ALA 174 ATOM 148 N HIS 175 ATOM 149 CA HIS 175 ATOM 151 CG HIS 175 ATOM 151 CG HIS 175 ATOM 153 ND1 HIS 175 ATOM 154 CE1 HIS 175 ATOM 155 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 157 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 157 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 157 NE2 HIS 175 ATOM 157 NE2 HIS 175 ATOM 156 NE2 HIS 175 ATOM 157 NE2 HIS 175		ATOM	117 CB VAL 170	52.816 27.120 7.384 1.00 21.33
ATOM 120 C VAL 170 54.891 28.477 7.521 1.00 20.58 ATOM 121 O VAL 170 54.926 29.704 7.554 1.00 22.32 ATOM 122 N ALA 171 55.712 27.696 8.230 1.00 18.83 ATOM 123 CA ALA 171 55.712 27.696 8.230 1.00 18.83 ATOM 124 CB ALA 171 55.712 27.696 8.230 1.00 18.34 ATOM 124 CB ALA 171 56.692 28.234 9.182 1.00 18.34 ATOM 125 C ALA 171 57.375 27.102 9.946 1.00 17.05 ATOM 126 O ALA 171 58.084 30.200 9.091 1.00 18.67 ATOM 127 N THR 172 58.231 28.756 7.367 1.00 17.84 ATOM 129 CB THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 129 CB THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 130 OG1 THR 172 60.280 27.531 5.776 1.00 20.47 ATOM 131 CG2 THR 172 58.655 30.932 6.251 1.00 19.42 ATOM 133 O THR 172 59.320 31.957 6.435 1.00 17.98 ATOM 134 N GLU 173 57.425 30.970 5.756 1.00 19.97 ATOM 135 CA GLU 173 56.811 32.236 5.374 1.00 22.51 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 22.51 ATOM 139 OE1 GLU 173 55.690 34.040 3.020 1.00 39.54 ATOM 139 OE1 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 140 OE2 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 140 OE2 GLU 173 56.638 33.099 6.622 1.00 21.60 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 144 CA ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 145 CB ALA 174 55.843 33.155 8.968 1.00 18.07 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 60.938 33.318 10.043 1.00 11.09 ATOM 150 CB HIS 175 60.938 33.318 10.043 1.00 11.09 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 154 CEI HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 62.373 34.252 10.920 1.00 18.26 ATOM 155 NE2 HIS 175 64.076 33.683 9.658 1.00 12.70		ATOM	118 CG1 VAL 170	52.224 28.113 8.366 1.00 22.32
ATOM 121 O VAL 170 54,926 29,704 7.554 1.00 22.32 ATOM 122 N ALA 171 55,712 27,696 8.230 1.00 18.83 ATOM 123 CA ALA 171 55,712 27,696 8.230 1.00 18.83 ATOM 124 CB ALA 171 57,375 27,102 9,946 1.00 17.05 ATOM 125 C ALA 171 57,375 27,102 9,946 1.00 17.05 ATOM 126 O ALA 171 58,084 30,200 9.091 1.00 18.67 ATOM 127 N THR 172 58,084 30,200 9.091 1.00 18.67 ATOM 128 CA THR 172 58,084 30,200 9.091 1.00 18.67 ATOM 129 CB THR 172 59,215 29,551 6.639 1.00 18.88 ATOM 130 OG1 THR 172 59,215 29,551 6.639 1.00 18.88 ATOM 130 OG1 THR 172 58,655 30,932 6.251 1.00 20,47 ATOM 131 CG2 THR 172 58,655 30,932 6.251 1.00 19,42 ATOM 134 N GLU 173 57,425 30,970 5,756 1.00 19,42 ATOM 135 CA GLU 173 56,811 32,236 5,374 1.00 22,51 ATOM 136 CB GLU 173 56,811 32,236 5,374 1.00 27,26 ATOM 139 OE1 GLU 173 56,610 33,454 4.005 1.00 34,96 ATOM 140 OE2 GLU 173 56,538 33.099 6.622 1.00 21,60 ATOM 141 C GLU 173 56,123 32,461 7,716 1.00 19,69 ATOM 144 CA ALA 174 ATOM 145 CB ALA 174 55,423 32,169 10,037 1.00 16,90 ATOM 146 C ALA 174 ATOM 146 C ALA 174 ATOM 147 O ALA 174 ATOM 148 N HIS 175 58,240 33,254 2,259 1.00 16,39 ATOM 149 CA HIS 175 60,574 32,758 9.804 1.00 12,71 ATOM 150 CB HIS 175 61,938 33,318 10,043 1.00 11,09 ATOM 150 CB HIS 175 62,373 34,252 10,920 1.00 8,26 ATOM 153 NDI HIS 175 63,030 32,977 9,273 1.00 13,39 ATOM 154 CEI HIS 175 64,076 33,683 9,658 1.00 12,70 ATOM 155 NE2 HIS 175 63,702 34,464 10,658 1.00 12,70		ATOM	119 CG2 VAL 170	51.740 26.608 6.438 1.00 23.27
ATOM 122 N ALA 171 55.712 27.696 8.230 1.00 18.83 ATOM 123 CA ALA 171 56.692 28.234 9.182 1.00 18.34 ATOM 124 CB ALA 171 57.375 27.102 9.946 1.00 17.05 ATOM 125 C ALA 171 57.375 27.102 9.946 1.00 17.05 ATOM 126 O ALA 171 57.373 29.151 8.533 1.00 17.84 ATOM 127 N THR 172 58.231 28.756 7.367 1.00 17.81 ATOM 128 CA THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 129 CB THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 130 OG1 THR 172 60.280 27.531 5.776 1.00 20.47 ATOM 131 CG2 THR 172 60.806 29.599 4.648 1.00 20.47 ATOM 133 O THR 172 59.320 31.957 6.435 1.00 17.98 ATOM 134 N GLU 173 56.851 30.932 6.251 1.00 19.97 ATOM 135 CA GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 137 CG GLU 173 56.811 32.236 5.374 1.00 27.26 ATOM 139 OE1 GLU 173 55.690 34.040 3.020 1.00 39.54 ATOM 140 OE2 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 145 CB ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 145 CB ALA 174 56.123 32.461 7.716 1.00 19.80 ATOM 148 N HIS 175 58.443 33.155 8.968 1.00 18.07 ATOM 149 CA HIS 175 58.443 33.155 8.968 1.00 18.07 ATOM 149 CA HIS 175 58.443 33.223 9.259 1.00 16.90 ATOM 148 N HIS 175 58.440 33.227 9.259 1.00 16.39 ATOM 149 CA HIS 175 58.498 33.831 9.629 1.00 16.41 ATOM 149 CA HIS 175 60.574 32.758 9.804 1.00 12.71 ATOM 150 CB HIS 175 60.373 34.252 10.920 1.00 8.26 ATOM 151 CG HIS 175 60.370 34.464 10.658 1.00 12.70 ATOM 154 CEI HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM	120 C VAL 170	54.891 28.477 7.521 1.00 20.58
ATOM 123 CA ALA 171 56.692 28.234 9.182 1.00 18.34 ATOM 124 CB ALA 171 57.375 27.102 9.946 1.00 17.05 ATOM 125 C ALA 171 57.733 29.151 8.533 1.00 17.84 20 ATOM 126 O ALA 171 58.084 30.200 9.091 1.00 18.67 ATOM 127 N THR 172 58.231 28.756 7.367 1.00 17.81 ATOM 128 CA THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 129 CB THR 172 59.215 29.551 6.639 1.00 18.88 ATOM 130 OG1 THR 172 60.280 27.531 5.776 1.00 20.47 ATOM 131 CG2 THR 172 60.806 29.599 4.648 1.00 20.22 ATOM 132 C THR 172 59.320 31.957 6.435 1.00 17.98 ATOM 134 N GLU 173 57.425 30.970 5.756 1.00 19.97 ATOM 136 CB GLU 173 56.811 32.236 5.374 1.00 22.51 ATOM 137 CG GLU 173 55.823 33.244 4.005 1.00 34.96 ATOM 138 CD GLU 173 55.690 34.040 3.020 1.00 39.54 ATOM 140 OE2 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 141 C GLU 173 56.518 33.099 6.622 1.00 21.60 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 ATOM 148 N HIS 175 58.493 33.244 1.00 12.71 45 ATOM 146 C ALA 174 55.423 32.169 10.037 1.00 16.90 ATOM 148 N HIS 175 58.493 33.318 10.043 1.00 11.09 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 ATOM 151 CG HIS 175 60.370 34.646 10.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	15	ATOM	121 O VAL 170	54.926 29.704 7.554 1.00 22.32
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ATOM 137 CG GLU 173 54.823 33.244 4.005 1.00 34.96 ATOM 138 CD GLU 173 55.690 34.040 3.020 1.00 39.54 ATOM 139 OE1 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 140 OE2 GLU 173 55.443 35.259 2.872 1.00 41.06 35 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	20			
ATOM 138 CD GLU 173 55.690 34.040 3.020 1.00 39.54 ATOM 139 OE1 GLU 173 56.610 33.454 2.395 1.00 41.82 ATOM 140 OE2 GLU 173 55.443 35.259 2.872 1.00 41.06 35 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	30			
ATOM 140 OE2 GLU 173 55.643 33.454 2.395 1.00 41.82 ATOM 140 OE2 GLU 173 55.443 35.259 2.872 1.00 41.06 35 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
ATOM 140 OE2 GLU 173 55.443 35.259 2.872 1.00 41.06 ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
ATOM 141 C GLU 173 56.538 33.099 6.622 1.00 21.60 ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
ATOM 142 O GLU 173 56.726 34.313 6.595 1.00 21.73 ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	35			
ATOM 143 N ALA 174 56.123 32.461 7.716 1.00 19.69 ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	55			
ATOM 144 CA ALA 174 55.844 33.155 8.968 1.00 18.07 ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
ATOM 145 CB ALA 174 55.423 32.169 10.037 1.00 16.90 40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
40 ATOM 146 C ALA 174 57.101 33.883 9.400 1.00 17.65 ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 150 CB HIS 175 69.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.37 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 12.70 <th></th> <th>ATOM</th> <th></th> <th></th>		ATOM		
ATOM 147 O ALA 174 57.052 35.031 9.829 1.00 19.80 ATOM 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	40	ATOM		
ATOM 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM		
ATOM 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM	148 N HIS 175	58.240 33.222 9.259 1.00 16.39
45 ATOM 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 155 NE2 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM	149 CA HIS 175	59.498 33.831 9.629 1.00 16.41
ATOM 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM	150 CB HIS 175	60.574 32.758 9.804 1.00 12.71
ATOM 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70	45	ATOM	151 CG HIS 175	61.938 33.318 10.043 1.00 11.09
ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70		ATOM	152 CD2 HIS 175	62.373 34.252 10.920 1.00 8.26
ATOM 155 NE2 HIS 175 63.702 34.464 10.658 1.00 12.70				
50 ATOM 156 C HIS 175 59.959 34.903 8.624 1.00 19.55				
	50	ATOM	156 C HIS 175	59.959 34.903 8.624 1.00 19.55

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157 O HIS 175
                              60.293 36.027 9.016 1.00 18.38
    ATOM
                               59.987 34.555 7.339 1.00 20.77
            158 N ARG 176
    ATOM
            159 CA ARG 176
                               60.424 35.494 6.307 1.00 21.30
    ATOM
                               60.315 34.876 4.917 1.00 24.87
    ATOM
            160 CB ARG 176
                               61.361 33.827 4.609 1.00 30.22
    ATOM
            161 CG ARG 176
                               61.429 33.603 3.116 1.00 36.29
    ATOM
            162 CD ARG 176
                               62.256 32.457 2.758 1.00 44.72
    ATOM
            163 NE ARG 176
            164 CZ ARG 176
                               62.031 31.680 1.700 1.00 49.80
    ATOM
                                61.000 31.935 0.894 1.00 50.83
            165 NH1 ARG 176
    ATOM
                                62.812 30.627 1.466 1.00 50.14
            166 NH2 ARG 176
10
    ATOM
                               59.658 36.807 6.337 1.00 20.67
    ATOM
            167 C ARG 176
                               60.256 37.877 6.238 1.00 20.53
    ATOM
            168 O ARG 176
    ATOM
            169 N SER 177
                              58.344 36.730 6.508 1.00 20.67
            170 CA SER 177
                               57.526 37.934 6.551 1.00 21.86
    ATOM
            171 CB SER 177
                               56.061 37.588 6.298 1.00 19.59
15
    ATOM
                               55.541 36.774 7.329 1.00 21.85
    ATOM
            172 OG SER 177
                              57.659 38.733 7.857 1.00 23.27
    ATOM
            173 C SER 177
                              57.073 39.807 7.989 1.00 24.40
    ATOM
            174 O SER 177
    ATOM
            175 N THR 178
                              58.383 38.202 8.837 1.00 22.16
                               58.542 38.913 10.095 1.00 20.62
20
    ATOM
            176 CA THR 178
            177 CB THR 178
                               57.853 38.162 11.265 1.00 19.93
    ATOM
            178 OG1 THR 178
                                58.386 36.838 11.381 1.00 18.72
    ATOM
            179 CG2 THR 178
                                56.359 38.057 11.033 1.00 16.95
    ATOM
            180 C THR 178
                              60.015 39.137 10.394 1.00 21.57
    ATOM
                              60.368 39.649 11.449 1.00 23.91
25
    ATOM
            181 O THR 178
                              60.870 38.769 9.445 1.00 22.22
    ATOM
            182 N ASN 179
                               62.316 38.912 9.585 1.00 24.22
    ATOM
            183 CA ASN 179
            184 CB ASN 179
                               63.013 37.690 8.970 1.00 22.49
    ATOM
                               64.480 37.596 9.344 1.00 23.53
            185 CG ASN 179
    ATOM
    ATOM
            186 OD1 ASN 179
                                64.866 37.912 10.464 1.00 22.32
30
                                65.296 37.100 8.425 1.00 23.84
    ATOM
            187 ND2 ASN 179
                              62.744 40.210 8.881 1.00 26.52
    ATOM
            188 C ASN 179
    ATOM
            189 O ASN 179
                              62.923 40.253 7.657 1.00 26.65
                              62.898 41.267 9.671 1.00 27.47
    ATOM
            190 N ALA 180
                               63.255 42.582 9.166 1.00 30.30
35
    ATOM
            191 CA ALA 180
                               63.552 43.508 10.321 1.00 27.21
    ATOM
            192 CB ALA 180
            193 C ALA 180
                              64.404 42.593 8.166 1.00 33.14
    ATOM
                               65,440 41.972 8.397 1.00 33.71
    ATOM
            194 O ALA 180
                               64.209 43.295 7.049 0.50 35.09
                                                             ALTA
    ATOM
            195 N GLN 181
            196 CA GLN 181
                               65.212 43.423 5.980 0.50 37.44
                                                             ALTA
40
    ATOM
            197 CB GLN 181
                               66.544 43.974 6.511 0.50 38.60
                                                             ALTA
    ATOM
            198 CG GLN 181
                               66,728 45.462 6.299 0.50 40.53
                                                             ALTA
    ATOM
    ATOM
            199 CD GLN 181
                               65.805 46.291 7.162 0.50 42.72
                                                              ALTA
    ATOM
            200 OE1 GLN 181
                                64.639 46.512 6.828 0.50 42.05
                                                              ALTA
            201 NE2 GLN 181
                                66.324 46.756 8.284 0.50 44.59
                                                              ALTA
45
    ATOM
            202 C GLN 181
                              65.481 42.180 5.138 0.50 38.43
                                                             ALTA
    ATOM
                                                             ALTA
            203 O GLN 181
                              66.175 42.262 4.118 0.50 38.92
    ATOM
            204 N GLY 182
                              64.958 41.034 5.562 1.00 38.74
    ATOM
            205 CA GLY 182
                               65.166 39.808 4.805 1.00 40.07
    ATOM
            206 C GLY 182
                              66.634 39.554 4.486 1.00 42.06
50
    ATOM
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	ATOM	207 O GLY 182	67.504 39.684 5.346 1.00 43.28	
	ATOM	208 N SER 183	66.926 39.272 3.224 1.00 43.72	
	ATOM	209 CA SER 183	68.299 39.001 2.812 1.00 45.88	
	ATOM	210 CB SER 183	68.304 38.069 1.593 1.00 47.26	
5	ATOM	211 OG SER 183	67.519 38.605 0.531 1.00 47.23	
	ATOM	212 C SER 183	69.095 40.268 2.497 1.00 46.24	
	ATOM	213 O SER 183	70.290 40.194 2.185 1.00 48.13	
	ATOM		68.445 41.426 2.579 1.00 45.79	
	ATOM		69.111 42.690 2.276 1.00 45.00	
10	ATOM	216 CB HIS 184		
- 0	ATOM		69.732 43.351 3.516 1.00 44.67	
	ATOM		70.316 44.440 3.428 1.00 45.02	
	ATOM	219 N TRP 185	69.659 42.663 4.653 1.00 43.24	
	ATOM	220 CA TRP 185	70.190 43.172 5.919 1.00 40.98	
15	ATOM	221 CB TRP 185	70.078 42.106 7.020 1.00 37.96	
13	ATOM	222 CG TRP 185	70.889 40.874 6.775 1.00 34.14	
	ATOM	223 CD2 TRP 185	72.197 40.593 7.291 1.00 33.38	
	ATOM	224 CE2 TRP 185	72.572 39.321 6.807 1.00 31.68	
	ATOM	225 CE3 TRP 185	73.092 41.296 8.107 1.00 31.65	
20	ATOM	226 CD1 TRP 185	70.530 39.790 6.028 1.00 34.27	
	ATOM	227 NE1 TRP 185	71.536 38.852 6.043 1.00 33.51	
	ATOM	228 CZ2 TRP 185	73.795 38.733 7.121 1.00 31.67	
	ATOM	229 CZ3 TRP 185	74.308 40.713 8.419 1.00 31.29	
	ATOM	230 CH2 TRP 185	74.651 39.444 7.923 1.00 31.06	
25	ATOM	231 C TRP 185	71.618 43.720 5.856 1.00 41.52	
	ATOM	232 O TRP 185	71.893 44.817 6.335 1.00 40.52	
	ATOM	233 N LYS 186	72.520 42.976 5.234 1.00 42.94	
	ATOM	234 CA LYS 186	73.896 43.417 5.143 1.00 45.25	
	ATOM		74.764 42.328 4.508 1.00 45.96	
30	ATOM	236 CG LYS 186	76.255 42.600 4.590 1.00 48.07	
	ATOM	237 CD LYS 186	77.053 41.307 4.504 1.00 51.20	
	ATOM	238 CE LYS 186	78.554 41.574 4.457 1.00 52.69	
	ATOM	239 NZ LYS 186	78.975 42.277 3.201 1.00 55.56	
	ATOM	240 C LYS 186	74.025 44.730 4.377 1.00 47.38	
35	ATOM	241 O LYS 186	74.914 45.535 4.663 1.00 47.65	
	ATOM	242 N GLN 187	73.134 44.959 3.418 0.50 48.02	ALTA
	ATOM	243 CA GLN 187	73.193 46.183 2.623 0.50 48.69	ALTA
	ATOM	244 CB GLN 187	72.547 45.973 1.246 0.50 48.66	ALTA
	ATOM	245 CG GLN 187	73.104 44.771 0.453 0.50 49.05	ALTA
40	ATOM	246 CD GLN 187	74.624 44.766 0.339 0.50 49.17	ALTA
	ATOM	247 OE1 GLN 187	75.225 45.691 -0.209 0.50 49.71	ALTA
	ATOM	248 NE2 GLN 187	75.250 43.710 0.847 0.50 48.57	ALTA
	ATOM	249 C GLN 187	72.551 47.373 3.343 0.50 49.06	ALTA
	ATOM	250 O GLN 187	73.094 48.475 3.329 0.50 49.53	ALTA
45	ATOM	251 N ARG 188	71.405 47.152 3.980 1.00 49.18	
	ATOM	252 CA ARG 188	70.723 48.221 4.695 1.00 49.90	
	ATOM	253 CB ARG 188	69.209 47.988 4.653 1.00 53.68	
	ATOM	254 CG ARG 188	68.617 47.798 3.251 1.00 57.22	
	ATOM	255 CD ARG 188	67.099 47.962 3.302 1.00 60.67	
50	ATOM	256 NE ARG 188	66.430 47.441 2.110 1.00 64.43	

	ATOM	257 CZ ARG 188	65.931 46.208 2.009 1.00 66.13
	ATOM	258 NH1 ARG 188	66.027 45.362 3.031 1.00 66.69
	ATOM	259 NH2 ARG 188	65.318 45.823 0.893 1.00 66.10
	ATOM	260 C ARG 188	71.150 48.510 6.133 1.00 48.42
5	ATOM	261 O ARG 188	70.544 49.368 6.784 1.00 48.86
	ATOM	262 N ARG 189	72.153 47.804 6.647 1.00 46.00
	ATOM	263 CA ARG 189	72.581 48.030 8.028 1.00 44.24
	ATOM	264 CB ARG 189	73.039 46.726 8.690 1.00 43.40
	ATOM	265 CG ARG 189	74.367 46.204 8.203 1.00 43.05
10	ATOM	266 CD ARG 189	74.808 45.021 9.019 1.00 43.62
	ATOM	267 NE ARG 189	76.185 44.660 8.717 1.00 45.95
	ATOM	268 CZ ARG 189	76.981 43.976 9.536 1.00 48.56
	ATOM	269 NH1 ARG 189	76.548 43.560 10.724 1.00 46.34
	ATOM	270 NH2 ARG 189	78.233 43.735 9.174 1.00 50.12
15	ATOM	271 C ARG 189	73.642 49.116 8.238 1.00 43.20
	ATOM	272 O ARG 189	74.629 49.210 7.500 1.00 43.07
	ATOM	273 N LYS 190	73.427 49.925 9.268 1.00 41.56
	ATOM	274 CA LYS 190	74.335 51.003 9.628 1.00 39.96
	ATOM	275 CB LYS 190	73.563 52.323 9.757 1.00 38.85
20	ATOM	276 C LYS 190	74.983 50.631 10.956 1.00 38.91
	ATOM	277 O LYS 190	74.345 50.015 11.806 1.00 38.17
	ATOM	278 N PHE 191	76.261 50.959 11.104 1.00 38.49
	ATOM	279 CA PHE 191	76.998 50.673 12.326 1.00 38.42
	ATOM	280 CB PHE 191	78.500 50.762 12.073 1.00 38.37
25	ATOM	281 CG PHE 191	79.056 49.608 11.308 1.00 39.05
	ATOM	282 CD1 PHE 191	78.712 49.408 9.976 1.00 40.02
	ATOM	283 CD2 PHE 191	79.942 48.727 11.917 1.00 39.19
	ATOM	284 CE1 PHE 191	79.245 48.344 9.256 1.00 40.57
	ATOM	285 CE2 PHE 191	80.482 47.661 11.213 1.00 40.32
30	ATOM	286 CZ PHE 191	80.133 47.466 9.875 1.00 41.84
	ATOM	287 C PHE 191	76.650 51.673 13.416 1.00 37.96
	ATOM	288 O PHE 191	76.568 52.872 13.151 1.00 38.95
	ATOM	289 N LEU 192	76.433 51.184 14.634 1.00 37.05
	ATOM	290 CA LEU 192	76.138 52.063 15.759 1.00 35.99
35	ATOM	291 CB LEU 192	75.833 51.247 17.014 1.00 33.04
	ATOM	292 CG LEU 192	75.503 52.074 18.260 1.00 31.38
	ATOM	293 CD1 LEU 192	74.116 52.651 18.102 1.00 29.02
	ATOM	294 CD2 LEU 192	75.592 51.229 19.536 1.00 30.32
	ATOM	295 C LEU 192	77.436 52.831 15.976 1.00 36.99
40	ATOM	296 O LEU 192	78.500 52.218 16.112 1.00 37.66
	ATOM	297 N PRO 193	77.377 54.177 15.988 1.00 38.15
	ATOM	298 CD PRO 193	76.156 54.996 15.902 1.00 37.90
	ATOM	299 CA PRO 193	78.561 55.025 16.187 1.00 38.68
	ATOM	300 CB PRO 193	77.950 56.365 16.568 1.00 37.20
45	ATOM	301 CG PRO 193	76.711 56.397 15.758 1.00 37.08
	ATOM	302 C PRO 193	79.475 54.503 17.294 1.00 41.12
	ATOM	303 O PRO 193	79.005 54.129 18.367 1.00 42.26
	ATOM	304 N ASP 194	80.782 54.509 17.052 1.00 43.62
	ATOM	305 CA ASP 194	81.731 54.012 18.050 1.00 46.71
50	ATOM	306 CB ASP 194	83.131 53.938 17.470 1.00 49.32

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307 CG ASP 194
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    ATOM
                                83.539 51.726 16.719 1.00 53.18
            308 OD1 ASP 194
    ATOM
            309 OD2 ASP 194
                                82.981 53.268 15.227 1.00 55.10
    ATOM
                              81.769 54.743 19.386 1.00 47.12
            310 C ASP 194
    ATOM
                              82.158 54.163 20.403 1.00 48.16
            311 O ASP 194
    ATOM
                              81.389 56.015 19.386 1.00 47.54
            312 N ASP 195
    ATOM
                               81.382 56.791 20.620 1.00 48.68
    ATOM 313 CA ASP 195
                               81.180 58.285 20.322 1.00 50.76
            314 CB ASP 195
    ATOM
                               79.871 58.572 19.602 1.00 54.24
            315 CG ASP 195
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                                78.929 59.082 20.253 1.00 56.17
            316 OD1 ASP 195
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    ATOM
                                79.786 58.292 18.385 1.00 56.08
            317 OD2 ASP 195
    ATOM
                              80,304 56,274 21.580 1.00 47.63
            318 C ASP 195
    ATOM
                               80.294 56.621 22.772 1.00 49.07
    ATOM
            319 O ASP 195
            320 N ILE 196
                              79.400 55.444 21.065 1.00 44.87
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            321 CA ILE 196
                               78.330 54.890 21.888 1.00 42.53
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15
                               76.983 54.813 21.121 1.00 42.19
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            322 CB ILE 196
                               75.870 54.357 22.060 1.00 40.29
    ATOM
            323 CG2 ILE 196
                               76.635 56.191 20.535 1.00 41.32
            324 CG1 ILE 196
     ATOM
                               75.344 56.219 19.732 1.00 41.32
            325 CD1 ILE 196
    ATOM
    ATOM 326 C ILE 196
                              78.725 53.509 22.391 1.00 40.89
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     ATOM 327 O ILE 196
                              79.358 52.722 21.679 1.00 40.08
            328 N GLY 197
                               78.384 53.240 23.642 1.00 40.16
     ATOM
                                78.705 51.957 24.228 1.00 40.21
            329 CA GLY 197
     ATOM
            330 C GLY 197
                               80.066 51.907 24.879 1.00 40.18
     ATOM
                               80.512 50.839 25.267 1.00 40.55
            331 O GLY 197
25
     ATOM
            332 N GLN 198
                               80,718 53.057 25.029 1.00 41.25
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            333 CA GLN 198
                                82.038 53.111 25.664 1.00 40.94
     ATOM
                                83.041 53.823 24.738 1.00 39.51
            334 CB GLN 198
     ATOM
            335 C GLN 198
                               81.995 53.796 27.046 1.00 40.93
     ATOM
                               83.036 54.197 27.571 1.00 41.83
            336 O GLN 198
     ATOM
30
            337 N SER 199
                               80.806 53.859 27.654 1.00 39.68
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                                80.615 54.510 28.961 1.00 37.74
            338 CA SER 199
     ATOM
                                79.995 55.905 28.768 1.00 38.50
            339 CB SER 199
     ATOM
                                80.687 56.672 27.792 1.00 40.71
            340 OG SER 199
     ATOM
                               79.743 53.726 29.958 1.00 36.31
            341 C SER 199
35
     ATOM
                               78.719 54.228 30.436 1.00 35.69
            342 O SER 199
     ATOM
                               80.123 52.484 30.280 1.00 35.05
            343 N PRO 200
     ATOM
                                81.246 51.684 29.760 1.00 33.97
            344 CD PRO 200
     ATOM
                                79.313 51.715 31.228 1.00 35.89
            345 CA PRO 200
     ATOM
                                79.872 50.304 31.075 1.00 33.94
             346 CB PRO 200
     ATOM
40
                                81,297 50.532 30.708 1.00 33.31
             347 CG PRO 200
     ATOM
             348 C PRO 200
                               79.477 52.241 32.656 1.00 37.75
     ATOM
                               80.484 51.959 33.299 1.00 38.78
     ATOM
            349 O PRO 200
                              78.493 52.988 33.158 1.00 39.61
            350 N ILE 201
     ATOM
                               78.590 53.551 34.511 1.00 40.56
            351 CA ILE 201
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     ATOM
                               78.715 55.093 34.484 1.00 40.20
            352 CB ILE 201
     ATOM
                                80.125 55.501 34.082 1.00 41.06
     ATOM 353 CG2 ILE 201
                                77.690 55.694 33.532 1.00 40.98
     ATOM 354 CG1 ILE 201
                                77.969 57.147 33.205 1.00 44.31
            355 CD1 ILE 201
     ATOM
                              77.535 53.160 35.546 1.00 41.40
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     ATOM
            356 C ILE 201
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	4 TO) (267 O HE 201	77.768 53.313 36.751 1.00 42.09
	ATOM		
	ATOM	358 N VAL 202	76.365 52.701 35.104 1.00 41.42
	ATOM	359 CA VAL 202	75.325 52.293 36.053 1.00 40.70
	ATOM	360 CB VAL 202	73.913 52.292 35.422 1.00 38.44
5	ATOM	361 CG1 VAL 202	72.881 51.826 36.435 1.00 35.91
	ATOM	362 CG2 VAL 202	73.560 53.692 34.934 1.00 36.42
	ATOM	363 C VAL 202	75.687 50.917 36.622 1.00 41.64
	ATOM	364 O VAL 202	76.094 50.008 35.894 1.00 42.05
	ATOM	365 N SER 203	75.596 50.800 37.938 1.00 43.06
10	ATOM	366 CA SER 203	75.947 49.576 38.639 1.00 44.57
	ATOM	367 CB SER 203	75.916 49.842 40.154 1.00 46.82
	ATOM	368 OG SER 203	76,457 48,772 40.916 1.00 50.18
	ATOM	369 C SER 203	75.052 48.388 38.294 1.00 44.08
	ATOM	370 O SER 203	73.849 48.534 38.093 1.00 44.28
15	ATOM	371 N MET 204	75.656 47.210 38.231 1.00 43.11
15	ATOM	372 CA MET 204	74.930 45.980 37.963 1.00 43.12
	ATOM	373 CB MET 204	75.048 45.557 36.494 1.00 41.07
	ATOM	374 CG MET 204	74.126 46.320 35.554 1.00 36.96
	ATOM	375 SD MET 204	72.375 46.134 35.990 1.00 38.66
20	ATOM	376 CE MET 204	71.970 44.592 35.098 1.00 37.26
20	ATOM	377 C MET 204	75.561 44.943 38.866 1.00 43.68
	ATOM	378 O MET 204	76.784 44.817 38.912 1.00 44.32
	ATOM	379 N PRO 205	74.735 44.204 39.619 1.00 44.22
	ATOM	380 CD PRO 205	73.261 44.310 39.610 1.00 44.44
25	ATOM	381 CA PRO 205	75.187 43.164 40.546 1.00 44.32
2,7	ATOM	382 CB PRO 205	73.944 42.299 40.701 1.00 45.18
	ATOM	383 CG PRO 205	72.832 43.335 40.691 1.00 44.29
	ATOM	384 C PRO 205	76.417 42.354 40.122 1.00 44.31
	ATOM	385 O PRO 205	77.393 42.293 40.864 1.00 43.97
30	ATOM	386 N ASP 206	76.404 41.802 38.912 1.00 44.30
30	ATOM	387 CA ASP 206	77.524 40.984 38.433 1.00 44.77
	ATOM	388 CB ASP 206	77.073 40.106 37.270 1.00 47.12
	ATOM	389 CG ASP 206	76.503 40.912 36.120 1.00 49.73
	ATOM	390 OD1 ASP 206	76.992 42.039 35.863 1.00 49.65
25		390 OD1 ASP 200 391 OD2 ASP 206	75.553 40.416 35.478 1.00 51.96
35	ATOM		78.805 41.718 38.037 1.00 44.10
	ATOM		79.754 41.099 37.549 1.00 43.60
	ATOM		78.804 43.039 38.145 1.00 44.19
	ATOM	394 N GLY 207	
40	ATOM	395 CA GLY 207	80.001 43.785 37.803 1.00 43.51
40	ATOM	396 C GLY 207	80.041 44.425 36.433 1.00 43.29
	ATOM	397 O GLY 207	80.745 45.421 36.257 1.00 44.47
	ATOM	398 N ASP 208	79.363 43.845 35.446 1.00 42.45
	ATOM	399 CA ASP 208	79.347 44.436 34.106 1.00 41.51
	ATOM	400 CB ASP 208	78.915 43.402 33.070 1.00 42.91
45	ATOM	401 CG ASP 208	80.001 42.379 32.785 1.00 43.57
	ATOM	402 OD1 ASP 208	79.675 41.218 32.468 1.00 44.55
	ATOM	403 OD2 ASP 208	81.191 42.742 32.868 1.00 47.14
	ATOM	404 C ASP 208	78.378 45.606 34.143 1.00 40.78
	ATOM	405 O ASP 208	77.176 45.403 34.277 1.00 42.50
50	ATOM	406 N LYS 209	78.902 46.827 34.058 1.00 39.10

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78.071 48.033 34.150 1.00 37.23
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            407 CA LYS 209
                               78.910 49.211 34.681 1.00 37.29
            408 CB LYS 209
     ATOM
            409 C LYS 209
                               77.326 48.423 32.871 1.00 34.47
     ATOM
                               77.707 48.013 31.776 1.00 33.85
            410 O LYS 209
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                               76,275 49,228 33,028 1.00 33,30
            411 N VAL 210
     ATOM
                                75.448 49.684 31.907 1.00 31.78
            412 CA VAL 210
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                                73.929 49.618 32.235 1.00 29.51
            413 CB VAL 210
     ATOM
                                73.102 50.012 31.010 1.00 29.24
            414 CG1 VAL 210
     ATOM
                                73.541 48.237 32.698 1.00 29.84
            415 CG2 VAL 210
     ATOM
            416 C VAL 210
                               75.731 51.115 31.451 1.00 32.68
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     ATOM
                               75.845 52.033 32.264 1.00 32.69
            417 O VAL 210
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            418 N ASP 211
                               75.769 51.290 30.134 1.00 33.00
     ATOM
                               75.978 52.574 29.476 1.00 31.85
     ATOM
            419 CA ASP 211
            420 CB ASP 211
                               76.826 52.353 28.221 1.00 32.38
     ATOM
            421 CG ASP 211
                               77.019 53.612 27.386 1.00 31.88
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            422 OD1 ASP 211
                                78.123 53.768 26.843 1.00 32.78
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            423 OD2 ASP 211
                                76.079 54.412 27.208 1.00 32.32
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            424 C ASP 211
                               73.925 52.444 28.206 1.00 31.94
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            425 O ASP 211
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            426 N LEU 212
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     ATOM
            427 CA LEU 212
            428 CB LEU 212
                                72.440 55.736 30.470 1.00 32.41
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                                72.311 55.336 31.936 1.00 32.11
     ATOM
            429 CG LEU 212
     ATOM
            430 CD1 LEU 212
                                72.447 56.555 32.830 1.00 32.35
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     ATOM
            431 CD2 LEU 212
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            432 C LEU 212
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            433 O LEU 212
                               71.326 54.695 27.609 1.00 32.13
     ATOM
                               73.370 55.589 27.407 1.00 32.21
            434 N GLU 213
     ATOM
            435 CA GLU 213
                                73.144 56.007 26.028 1.00 33.12
     ATOM
     ATOM
            436 CB GLU 213
                                74.305 56.864 25.530 1.00 36.72
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            437 CG GLU 213
                                74.067 57.468 24.146 1.00 40.61
            438 CD GLU 213
                                75.316 58.101 23.545 1.00 44.21
     ATOM
                                76.434 57.851 24.059 1.00 46.23
            439 OE1 GLU 213
     ATOM
            440 OE2 GLU 213
                                75.178 58.836 22.543 1.00 45.81
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            441 C GLU 213
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     ATOM
            442 O GLU 213
                               72.064 54.775 24.273 1.00 31.31
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                               73.827 53.803 25.285 1.00 30.66
            443 N ALA 214
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                                73,769 52,585 24,482 1.00 30,43
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            445 CB ALA 214
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            447 O ALA 214
            448 N PHE 215
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                                69.443 50.689 28.535 1.00 25.53
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            451 CG PHE 215
                                69.330 49.344 28.854 1.00 26.16
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            452 CD1 PHE 215
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     ATOM
            453 CD2 PHE 215
                                68.144 48.831 29.370 1.00 25.73
     ATOM 454 CE1 PHE 215
            455 CE2 PHE 215
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     ATOM
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            456 CZ PHE 215
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             458 O PHE 215
                               68.773 51.107 25.316 1.00 30.38
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             459 N SER 216
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             460 CA SER 216
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            461 CB SER 216
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                                67.972 56.153 24.628 1.00 35.83
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            462 OG SER 216
            463 C SER 216
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     ATOM
                               67.527 53.235 23.129 1.00 31.34
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            464 O SER 216
            465 N GLU 217
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            466 CA GLU 217
                                69.823 53.121 21.609 1.00 33.06
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     ATOM
            467 CB GLU 217
                                71,269 53.153 21.110 1.00 34.93
     ATOM
            468 CG GLU 217
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                                70.986 55.399 19.963 1.00 41.92
            469 CD GLU 217
     ATOM
     ATOM
            470 OE1 GLU 217
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            471 OE2 GLU 217
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            472 C GLU 217
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            473 O GLU 217
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                               69.477 50.779 22.181 1.00 29.80
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            475 CA PHE 218
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            476 CB PHE 218
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            478 CD1 PHE 218
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            479 CD2 PHE 218
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            480 CE1 PHE 218
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            481 CE2 PHE 218
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     ATOM
            483 C PHE 218
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     ATOM
            487 CB THR 219
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            488 OG1 THR 219
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     ATOM
            489 CG2 THR 219
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     ATOM
            490 C THR 219
                               64.747 50.689 22.782 1.00 27.21
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     ATOM
            491 O THR 219
                               63,588 50,348 22,557 1.00 28,58
            492 N LYS 220
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            493 CA LYS 220
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     ATOM
            494 CB LYS 220
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            495 C LYS 220
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            496 O LYS 220
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            497 N ILE 221
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            498 CA ILE 221
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     ATOM
            499 CB ILE 221
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     ATOM
     ATOM
             500 CG2 ILE 221
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45
             501 CG1 ILE 221
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     ATOM
             502 CD1 ILE 221
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     ATOM
     ATOM
            503 C ILE 221
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                              63.552 47.678 18.076 1.00 28.59
            504 O ILE 221
     ATOM
            505 N ILE 222
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     ATOM
             506 CA ILE 222
                               63.279 46.934 20.665 1.00 27.22
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     ATOM
             508 CG2 ILE 222
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     ATOM
            509 CG1 ILE 222
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            510 CD1 ILE 222
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     ATOM
     ATOM
            511 C ILE 222
                              61.797 46.614 20.519 1.00 28.33
            512 O ILE 222
                              61.445 45.459 20.260 1.00 29.81
     ATOM
                               60.929 47.618 20.622 1.00 27.63
            513 N THR 223
     ATOM
            514 CA THR 223
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            515 CB THR 223
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                                 58.839 48.983 22.180 1.00 30.67
            516 OG1 THR 223
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     ATOM
                                 57.183 48.390 20.525 1.00 26.50
     ATOM
            517 CG2 THR 223
                               59.103 46.698 19.183 1.00 25.28
     ATOM
            518 C THR 223
            519 O THR 223
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     ATOM
            520 N PRO 224
                               59.535 47.256 18.031 1.00 23.96
            521 CD PRO 224
                                60.138 48.580 17.792 1.00 22.28
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     ATOM
            522 CA PRO 224
                                59.181 46.612 16.759 1.00 23.13
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             523 CB PRO 224
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            524 CG PRO 224
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            525 C PRO 224
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                               59.198 44.332 15.994 1.00 22.77
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     ATOM
            527 N ALA 225
                               60.960 44.989 17.240 1.00 19.17
            528 CA ALA 225
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                                63.009 43.773 17.806 1.00 16.79
            529 CB ALA 225
     ATOM
            530 C ALA 225
                               60.802 42.643 17.969 1.00 19.08
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            531 O ALA 225
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     ATOM
     ATOM
            532 N ILE 226
                              60.253 43.033 19.117 1.00 18.30
                               59.420 42.147 19.929 1.00 18.65
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            533 CA ILE 226
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            534 CB ILE 226
                               59.092 42.779 21.288 1.00 17.30
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            535 CG2 ILE 226
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            536 CG1 ILE 226
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            537 CD1 ILE 226
            538 C ILE 226
     ATOM
                              58.109 41.858 19.199 1.00 19.56
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            539 O ILE 226
                              57.638 40.719 19.163 1.00 19.51
     ATOM
            540 N THR 227
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     ATOM
            541 CA THR 227
                                56.278 42.782 17.881 1.00 21.19
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            543 OG1 THR 227
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            544 CG2 THR 227
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            545 C THR 227
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            546 O THR 227
                               55.487 40.978 16.496 1.00 21.18
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            547 N ARG 228
            548 CA ARG 228
                                57.783 40.786 14.991 1.00 18.29
     ATOM
            549 CB ARG 228
                                59.032 41.136 14.191 1.00 19.95
     ATOM
            550 CG ARG 228
                                58.810 42.349 13.286 1.00 23.31
     ATOM
                                60.001 42.646 12.405 1.00 25.64
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     ATOM
            551 CD ARG 228
                                61.139 43.138 13.171 1.00 27.01
     ATOM
            552 NE ARG 228
     ATOM
            553 CZ ARG 228
                                62.209 42.413 13.468 1.00 28.20
     ATOM
            554 NH1 ARG 228
                                 62.280 41.155 13.067 1.00 28.99
            555 NH2 ARG 228
                                 63.219 42.951 14.141 1.00 27.25
     ATOM
                               57.834 39.352 15.502 1.00 18.40
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            556 C ARG 228
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	ATOM	557 O ARG 228	57.433 38.431 14.788 1.00 17.50
	ATOM	558 N VAL 229	58.278 39.162 16.747 1.00 17.42
	ATOM	559 CA VAL 229	58.316 37.822 17.334 1.00 16.40
	ATOM	560 CB VAL 229	59.116 37.779 18.674 1.00 15.88
5	ATOM	561 CG1 VAL 229	58.955 36.422 19.334 1.00 16.19
	ATOM	562 CG2 VAL 229	60.591 38.010 18.421 1.00 14.44
	ATOM	563 C VAL 229	56.852 37.408 17.552 1.00 16.75
	ATOM	564 O VAL 229	56.456 36.282 17.219 1.00 16.06
	ATOM	565 N VAL 230	56.039 38.343 18.046 1.00 16.09
10	ATOM	566 CA VAL 230	54.612 38.097 18.266 1.00 16.97
	ATOM	567 CB VAL 230	53.896 39.327 18.897 1.00 18.60
	ATOM	568 CG1 VAL 230	52.401 39.084 18.972 1.00 17.19
	ATOM	569 CG2 VAL 230	54.445 39.629 20.299 1.00 17.82
	ATOM	570 C VAL 230	53.938 37.780 16.916 1.00 18.46
15	ATOM	571 O VAL 230	53.115 36.863 16.828 1.00 18.46
	ATOM	572 N ASP 231	54.289 38.539 15.874 1.00 19.21
	ATOM	573 CA ASP 231	53.730 38.339 14.531 1.00 19.93
	ATOM	574 CB ASP 231	54.231 39.415 13.555 1.00 20.98
	ATOM	575 CG ASP 231	53.754 40.817 13.915 1.00 24.11
20	ATOM	576 OD1 ASP 231	52.704 40.953 14.586 1.00 24.23
	ATOM	577 OD2 ASP 231	54.443 41.784 13.522 1.00 25.90
	ATOM	578 C ASP 231	54.097 36.962 13.982 1.00 19.27
	ATOM	579 O ASP 231	53.266 36.279 13.380 1.00 17.80
	ATOM	580 N PHE 232	55.357 36.582 14.163 1.00 18.91
25	ATOM	581 CA PHE 232	55.841 35.288 13.712 1.00 19.65
	ATOM	582 CB PHE 232	57.308 35.078 14.104 1.00 18.14
	ATOM	583 CG PHE 232	57.752 33.639 14.027 1.00 19.70
	ATOM	584 CD1 PHE 232	57.895 33.005 12.799 1.00 19.18
	ATOM	585 CD2 PHE 232	57.987 32.904 15.188 1.00 17.61
30	ATOM	586 CE1 PHE 232	58.259 31.660 12.723 1.00 19.86
	ATOM	587 CE2 PHE 232	58.350 31.560 15.126 1.00 18.98
	ATOM	588 CZ PHE 232	58.487 30.935 13.892 1.00 19.46
	ATOM	589 C PHE 232	54.996 34.179 14.320 1.00 21.02
	ATOM	590 O PHE 232	54.458 33.339 13.598 1.00 20.88
35	ATOM	591 N ALA 233	54.863 34.202 15.645 1.00 21.64
	ATOM	592 CA ALA 233	54.106 33.187 16.378 1.00 21.43
	ATOM	593 CB ALA 233	54.223 33.443 17.868 1.00 18.72
	ATOM	594 C ALA 233	52.643 33.134 15.955 1.00 23.15
	ATOM	595 O ALA 233	52.043 32.062 15.857 1.00 21.76
40	ATOM	596 N LYS 234	52.083 34.307 15.689 1.00 25.54
	ATOM	597 CA LYS 234	50.695 34.446 15.273 1.00 27.57
	ATOM	598 CB LYS 234	50.360 35.935 15.146 1.00 30.65
	ATOM	599 CG LYS 234	49.110 36.349 15.867 1.00 36.27
	ATOM	600 CD LYS 234	49.192 35.988 17.334 1.00 41.19
45	ATOM	601 CE LYS 234	47.800 35.677 17.890 1.00 43.69
	ATOM	602 NZ LYS 234	47.119 34.565 17.147 1.00 44.98
	ATOM	603 C LYS 234	50.443 33.739 13.933 1.00 27.70
	ATOM	604 O LYS 234	49.355 33.200 13.693 1.00 28.42
	ATOM	605 N LYS 235	51.458 33.732 13.074 1.00 26.06
50	ATOM	606 CA LYS 235	51.364 33.113 11.758 1.00 26.47

	ATOM	607 CB LYS 235	52.350 33.791 10.819 1.00 25.23
	ATOM	608 CG LYS 235	52.051 35.269 10.644 1.00 26.92
	ATOM	609 CD LYS 235	53.017 35.959 9.697 1.00 28.41
	ATOM	610 CE LYS 235	52.500 37.350 9.318 1.00 29.31
5	ATOM	611 NZ LYS 235	53.400 38.026 8.347 1.00 30.37
•	ATOM	612 C LYS 235	51.540 31.588 11.722 1.00 27.93
	ATOM	613 O LYS 235	51.540 30.984 10.649 1.00 29.04
	ATOM	614 N LEU 236	51.718 30.973 12.887 1.00 28.83
	ATOM	615 CA LEU 236	51,866 29,524 12,986 1.00 29.05
10	ATOM	616 CB LEU 236	52,928 29.150 14.026 1.00 27.43
	ATOM	617 CG LEU 236	54.352 29.660 13.774 1.00 25.84
	ATOM	618 CD1 LEU 236	55.311 29.118 14.847 1.00 23.99
	ATOM	619 CD2 LEU 236	54.801 29.236 12.389 1.00 23.86
	ATOM	620 C LEU 236	50.513 28.948 13.392 1.00 31.19
15	ATOM	621 O LEU 236	49.870 29.435 14.328 1.00 31.48
	ATOM	622 N PRO 237	50.078 27.875 12.717 1.00 34.60
	ATOM	623 CD PRO 237	50.829 27.156 11.668 1.00 35.04
	ATOM	624 CA PRO 237	48,789 27.223 13.002 1.00 36.52
	ATOM	625 CB PRO 237	48.751 26.081 11.981 1.00 37.48
20	ATOM	626 CG PRO 237	50.229 25.776 11.718 1.00 36.60
	ATOM	627 C PRO 237	48.582 26.720 14.447 1.00 37.82
	ATOM	628 O PRO 237	47.629 27.102 15.125 1.00 37.08
	ATOM	629 N MET 238	49.495 25.893 14.935 1.00 40.42
	ATOM	630 CA MET 238	49.366 25.350 16.285 1.00 43.00
25	ATOM	631 CB MET 238	50.453 24.298 16.549 1.00 45.20
	ATOM	632 CG MET 238	50.043 22.837 16.296 1.00 47.16
	ATOM	633 SD MET 238	50.598 22.117 14.725 1.00 52.25
	ATOM	634 CE MET 238	52.305 21.809 15.033 1.00 47.29
	ATOM	635 C MET 238	49.389 26.389 17.414 1.00 43.25
30	ATOM	636 O MET 238	49.061 26.056 18.558 1.00 44.74
	ATOM	637 N PHE 239	49.720 27.642 17.088 1.00 41.55
	ATOM	638 CA PHE 239	49.825 28.716 18.091 1.00 37.31
	ATOM	639 CB PHE 239	51.031 29.615 17.765 1.00 32.40
25	ATOM	640 CG PHE 239	51.293 30.673 18.795 1.00 27.12
35	ATOM	641 CD1 PHE 239	52.099 30.398 19.893 1.00 24.57
	ATOM ATOM	642 CD2 PHE 239 643 CE1 PHE 239	50.705 31.933 18.686 1.00 24.70 52.319 31.356 20.876 1.00 25.09
	ATOM	644 CE2 PHE 239	50.915 32.901 19.659 1.00 25.90
	ATOM	645 CZ PHE 239	51.726 32.612 20.761 1.00 24.52
40	ATOM	646 C PHE 239	48.574 29.582 18.352 1.00 36.84
70	ATOM	647 O PHE 239	48.136 29.728 19.497 1.00 34.67
	ATOM	648 N SER 240	48.027 30.180 17.299 1.00 36.92
	ATOM	649 CA SER 240	.46.857 31.038 17.433 1.00 37.16
	ATOM	650 CB SER 240	46.534 31.706 16.094 1.00 38.34
45	ATOM	651 C SER 240	45.627 30.304 17.981 1.00 37.30
	ATOM	652 O SER 240	44.680 30.941 18.433 1.00 36.95
	ATOM	653 N GLU 241	45.639 28.974 17.917 1.00 37.73
	ATOM	654 CA GLU 241	44.531 28.155 18.418 1.00 38.44
	ATOM	655 CB GLU 241	44.644 26.705 17.912 1.00 42.18
50	ATOM	656 CG GLU 241	44.290 26.471 16.436 1.00 48.01

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		44 OD OLI 041	44.550.05.000.15.070.1.00.50.10
	ATOM	657 CD GLU 241	44.559 25.028 15.973 1.00 50.12
	ATOM	658 OE1 GLU 241	44.375 24.088 16.779 1.00 51.14
	ATOM	659 OE2 GLU 241	44.957 24.838 14.799 1.00 50.68
_	ATOM	660 C GLU 241	44.571 28.122 19.937 1.00 35.85
5	ATOM	661 O GLU 241	43.561 27.868 20.598 1.00 36.01
	ATOM	662 N LEU 242	45.762 28.329 20.480 1.00 33.28
	ATOM	663 CA LEU 242	45.959 28.296 21.920 1.00 31.31
	ATOM	664 CB LEU 242	47.452 28.382 22.244 1.00 29.28
	ATOM	665 CG LEU 242	48.318 27.202 21.797 1.00 29.95
10	ATOM	666 CD1 LEU 242	49.771 27.538 22.025 1.00 29.19
	ATOM	667 CD2 LEU 242	47.935 25.931 22.564 1.00 29.57
	ATOM	668 C LEU 242	45.223 29.390 22.676 1.00 30.10
	ATOM	669 O LEU 242	44.874 30.434 22.116 1.00 28.69
	ATOM	670 N PRO 243	44.867 29.115 23.937 1.00 30.09
15	ATOM	671 CD PRO 243	44.783 27.843 24.674 1.00 28.53
	ATOM	672 CA PRO 243	44.183 30.200 24.640 1.00 31.01
	ATOM	673 CB PRO 243	43.829 29.577 26.005 1.00 30.34
	ATOM	674 CG PRO 243	44.640 28.300 26.093 1.00 29.25
	ATOM	675 C PRO 243	45.195 31.356 24.774 1.00 31.71
20	ATOM	676 O PRO 243	46.412 31.128 24.840 1.00 30.69
	ATOM	677 N CYS 244	44.694 32.585 24.804 1.00 32.36
	ATOM	678 CA CYS 244	45.539 33.763 24.920 1.00 33.57
	ATOM	679 CB CYS 244	44.675 35.028 25.050 1.00 37.62
	ATOM	680 SG CYS 244	45.262 36.418 24.022 1.00 51.95
25	ATOM	681 C CYS 244	46.536 33.660 26.081 1.00 31.12
	ATOM	682 O CYS 244	47.677 34.087 25.942 1.00 30.37
	ATOM	683 N GLU 245	46.124 33.045 27.194 1.00 30.00
	ATOM	684 CA GLU 245	46.993 32.877 28.366 1.00 29.62
30	ATOM	685 CB GLU 245	46.270 32.159 29.514 1.00 33.10
30	ATOM	686 CG GLU 245	45.325 33.018 30.333 1.00 36.43
	ATOM	687 CD GLU 245	43.882 32.940 29.860 1.00 37.87
	ATOM	688 OE1 GLU 245	42.989 33.006 30.730 1.00 37.36
	ATOM	689 OE2 GLU 245	43.639 32.813 28.634 1.00 39.63
25	ATOM	690 C GLU 245	48.239 32.077 28.030 1.00 28.34
35	ATOM	691 O GLU 245	49.322 32.343 28.557 1.00 27.88
	ATOM	692 N ASP 246	48.063 31.043 27.213 1.00 26.10 49.182 30.212 26.798 1.00 25.23
	ATOM ATOM	693 CA ASP 246 694 CB ASP 246	,,,,,,
			48.685 28.923 26.135 1.00 26.98
40	ATOM	695 CG ASP 246	48.146 27.912 27.137 1.00 29.13
40	ATOM	696 OD1 ASP 246	48.158 28.193 28.354 1.00 26.52
	ATOM	697 OD2 ASP 246	47.712 26.824 26.696 1.00 31.38 50.065 30.983 25.826 1.00 23.57
	ATOM	698 C ASP 246	
	ATOM	699 O ASP 246	51.288 30.993 25.955 1.00 22.61
1 F	ATOM	700 N GLN 247	49.431 31.630 24.852 1.00 23.23
45	ATOM	701 CA GLN 247	50.144 32.408 23.855 1.00 22.20
	ATOM	702 CB GLN 247	49.159 33.178 22.991 1.00 22.06 48.329 32.307 22.066 1.00 22.74
	ATOM	703 CG GLN 247	
	ATOM	704 CD GLN 247 705 OE1 GLN 247	47.435 33.141 21.169 1.00 24.91 47.860 34.160 20.625 1.00 26.30
50	ATOM		46.186 32.732 21.035 1.00 25.65
50	ATOM	706 NE2 GLN 247	40.160 32.732 21.033 1.00 23.03

	4 TO) 4	707 C GLN 247	E1 000 22 274 24 520 1 00 22 10
	ATOM		51.098 33.374 24.528 1.00 22.10
	ATOM	708 O GLN 247	52.280 33.454 24.182 1.00 23.07
	ATOM	709 N ILE 248	50.587 34.076 25.527 1.00 23.27
_	ATOM	710 CA ILE 248	51.379 35.042 26.276 1.00 23.21
5	ATOM	711 CB ILE 248	50.473 35.824 27.273 1.00 24.59
	ATOM	712 CG2 ILE 248	51.304 36.682 28.242 1.00 24.09
	ATOM	713 CG1 ILE 248	49.499 36.707 26.487 1.00 23.47
	ATOM	714 CD1 ILE 248	48.413 37.323 27.341 1.00 23.84
	ATOM	715 C ILE 248	52.568 34.387 26.986 1.00 22.27
10	ATOM	716 O ILE 248	53.705 34.833 26.829 1.00 22.06
	ATOM	717 N ILE 249	52.321 33.313 27.729 1.00 21.40
	ATOM	718 CA ILE 249	53.398 32.630 28.440 1.00 21.40
	ATOM	719 CB ILE 249	52.850 31.438 29.279 1.00 23.53
	ATOM	720 CG2 ILE 249	53.972 30.489 29.711 1.00 21.44
15	ATOM	721 CG1 ILE 249	52.098 31.963 30.500 1.00 22.76
	ATOM	722 CD1 ILE 249	51.252 30.911 31.175 1.00 25.03
	ATOM	723 C ILE 249	54.481 32.148 27.470 1.00 22.24
	ATOM	724 O ILE 249	55.677 32.321 27.733 1.00 22.90
	ATOM	725 N LEU 250	54.072 31.582 26.334 1.00 22.65
20	ATOM	726 CA LEU 250	55.028 31.079 25.345 1.00 21.40
	ATOM	727 CB LEU 250	54.319 30.290 24.239 1.00 20.06
	ATOM	728 CG LEU 250	53.566 29.038 24.677 1.00 20.22
	ATOM	729 CD1 LEU 250	52.952 28.406 23.453 1.00 19.19
	ATOM	730 CD2 LEU 250	54.494 28.050 25.386 1.00 18.52
25	ATOM	731 C LEU 250	55.850 32.209 24.736 1.00 20.82
	ATOM	732 O LEU 250	57.069 32.094 24.603 1.00 20.27
	ATOM	733 N LEU 251	55.179 33.302 24.384 1.00 22.14
	ATOM	734 CA LEU 251	55.842 34.467 23.805 1.00 22.90
	ATOM	735 CB LEU 251	54.806 35.543 23.471 1.00 22.76
30	ATOM	736 CG LEU 251	54.513 35.899 22.012 1.00 23.35
	ATOM	737 CD1 LEU 251	55.347 35.103 21.047 1.00 22.38
	ATOM	738 CD2 LEU 251	53.040 35.708 21.747 1.00 22.86
	ATOM	739 C LEU 251	56.891 35.030 24.776 1.00 23.67
	ATOM	740 O LEU 251	58.051 35.234 24.402 1.00 22.58
35	ATOM	741 N LYS 252	56.491 35.236 26.029 1.00 24.64
	ATOM	742 CA LYS 252	57.395 35.754 27.057 1.00 26.22
	ATOM	743 CB LYS 252	56.617 36.037 28.350 1.00 27.79
	ATOM	744 CG LYS 252	55.351 36.838 28.093 1.00 32.69
	ATOM	745 CD LYS 252	55.185 38.023 29.003 1.00 35.85
40	ATOM	746 CE LYS 252	54.773 37.626 30.397 1.00 39.34
	ATOM	747 NZ LYS 252	54.477 38.870 31.168 1.00 44.60
	ATOM	748 C LYS 252	58.566 34.793 27.312 1.00 25.26
	ATOM	749 O LYS 252	59.701 35.222 27.555 1.00 26.67
	ATOM	750 N GLY 253	58.306 33.497 27.195 1.00 23.97
45	ATOM	751 CA GLY 253	59.356 32.521 27.404 1.00 22.00
	ATOM	752 C GLY 253	60.397 32.429 26.292 1.00 23.10
	ATOM	753 O GLY 253	61.568 32.165 26.585 1.00 25.12
	ATOM	754 N CYS 254	60.014 32.702 25.041 1.00 22.27
	ATOM	755 CA CYS 254	60.944 32.584 23.908 1.00 20.91
50	ATOM	756 CB CYS 254	60.353 31.648 22.845 1.00 21.46

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58.992 32.385 21.893 1.00 22.92
             757 SG CYS 254
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             758 C CYS 254
     ATOM
                               62.215 33.834 22.316 1.00 19.88
             759 O CYS 254
     ATOM
                               60.731 34.984 23.561 1.00 19.56
             760 N CYS 255
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             761 CA CYS 255
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                                60.292 37.407 23.634 1.00 21.21
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                                60.404 38.957 22.735 1.00 22.22
            763 SG CYS 255
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                               62.504 36.590 22.775 1.00 21.36
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     ATOM
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             765 O CYS 255
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            766 N MET 256
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     ATOM
            767 CA MET 256
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             768 CB MET 256
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                                66.744 37.360 25.267 1.00 19.20
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             769 CG MET 256
             770 SD MET 256
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             771 CE MET 256
                                68.856 38.971 24.375 1.00 18.47
15
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             772 C MET 256
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             773 O MET 256
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                                65.035 34.568 23.170 1.00 19.00
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             774 N GLU 257
                                65.685 33.480 22.443 1.00 19.71
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             775 CA GLU 257
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     ATOM
             776 CB GLU 257
                                65.104 32.145 22.882 1.00 21.15
                                65.451 31.821 24.319 1.00 26.39
             777 CG GLU 257
     ATOM
             778 CD GLU 257
                                64.513 30.820 24.929 1.00 30.75
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            779 OEI GLU 257
                                 63.875 30.069 24.162 1.00 32.36
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                                 64.415 30.783 26.172 1.00 33.70
            780 OE2 GLU 257
     ATOM
             781 C GLU 257
                               65.545 33.648 20.940 1.00 18.54
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     ATOM
                                66.521 33.506 20.197 1.00 17.58
             782 O GLU 257
     ATOM
             783 N ILE 258
                              64.336 33.977 20.497 1.00 17.78
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             784 CA ILE 258
                               64.101 34.176 19.081 1.00 17.60
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             785 CB ILE 258
                               62.590 34.267 18.765 1.00 16.35
     ATOM
                                62.376 34.777 17.326 1.00 16.20
     ATOM
             786 CG2 ILE 258
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                                61.935 32.884 18.980 1.00 17.24
     ATOM
             787 CG1 ILE 258
             788 CD1 ILE 258
                                60.437 32.787 18.593 1.00 14.08
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                              64.872 35.408 18.595 1.00 19.11
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             789 C ILE 258
                              65.609 35.326 17.601 1.00 19.02
     ATOM
             790 O ILE 258
                                64.785 36.517 19.341 1.00 19.71
             791 N MET 259
35
     ATOM
            792 CA MET 259
793 CB MET 259
                                65.486 37.744 18.956 1.00 18.43
     ATOM
                                65.162 38.890 19.910 1.00 19.99
     ATOM
                                63,700 39,278 19,962 1,00 21,15
            794 CG MET 259
     ATOM
                                63.452 40.921 20.700 1.00 24.33
             795 SD MET 259
     ATOM
                                63.769 40.595 22.415 1.00 22.50
     ATOM
             796 CE MET 259
40
                                66.993 37.540 18.888 1.00 18.64
             797 C MET 259
     ATOM
             798 O MET 259
                                67.638 37.993 17.941 1.00 19.96
     ATOM
             799 N SER 260
                               67.556 36.858 19.884 1.00 17.37
     ATOM
                                68.993 36.592 19.915 1.00 16.76
     ATOM
             800 CA SER 260
                                69,387 35.840 21.195 1.00 17.25
     ATOM
             801 CB SER 260
45
                                69.078 36.589 22.346 1.00 22.89
     ATOM
             802 OG SER 260
             803 C SER 260
                               69.387 35.750 18.717 1.00 15.13
     ATOM
             804 O SER 260
                               70.460 35.941 18.137 1.00 16.62
     ATOM
                               68.539 34.781 18.385 1.00 15.15
             805 N LEU 261
     ATOM
             806 CA LEU 261
                                68.802 33.900 17.262 1.00 15.31
50
     ATOM
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	ATOM	807 CB LEU 261	67.708 32.834 17.153 1.00 15.43
	ATOM	808 CG LEU 261	67.652 32.014 15.858 1.00 15.82
	ATOM	809 CD1 LEU 261	68.963 31.251 15.621 1.00 16.35
	ATOM	810 CD2 LEU 261	66.470 31.060 15.937 1.00 13.72
5	ATOM	811 C LEU 261	68.839 34.741 16.001 1.00 16.31
_	ATOM	812 O LEU 261	69.766 34.619 15.194 1.00 16.68
	ATOM	813 N ARG 262	67.848 35.620 15.853 1.00 16.47
	ATOM	814 CA ARG 262	67.778 36.493 14.680 1.00 16.66
	ATOM	815 CB ARG 262	66.475 37.279 14.693 1.00 16.00
10	ATOM	816 CG ARG 262	65.291 36.404 14.354 1.00 15.62
10	ATOM	817 CD ARG 262	63.995 37.167 14.378 1.00 17.31
	ATOM	818 NE ARG 262	62.967 36.454 13.628 1.00 20.09
	ATOM:	819 CZ ARG 262	61.755 36.932 13.361 1.00 21.06
	ATOM	820 NH1 ARG 262	61.390 38.136 13.787 1.00 19.02
15	ATOM	821 NH2 ARG 262	60.909 36.207 12.640 1.00 22.63
13	ATOM	822 C ARG 262	69.003 37.396 14.527 1.00 16.80
	ATOM	823 O ARG 262	69.440 37.664 13.412 1.00 16.82
	ATOM	824 N ALA 263	69.578 37.832 15.650 1.00 17.77
	ATOM	825 CA ALA 263	70.795 38.647 15.637 1.00 18.41
20	ATOM	826 CB ALA 263	70.996 39.337 17.004 1.00 18.26
20	ATOM	827 C ALA 263	71.998 37.740 15.327 1.00 19.15
	ATOM	828 O ALA 263	72.837 38.063 14.475 1.00 19.40
	ATOM	829 N ALA 264	72.056 36.587 15.996 1.00 19.84
	ATOM	830 CA ALA 264	73.155 35.633 15.818 1.00 20.35
25	ATOM	831 CB ALA 264	73.045 34.483 16.832 1.00 18.09
	ATOM	832 C ALA 264	73.289 35.079 14.398 1.00 20.66
	ATOM	833 O ALA 264	74.406 34.870 13.922 1.00 21.04
	ATOM	834 N VAL 265	72.173 34.822 13.723 1.00 21.14
	ATOM	835 CA VAL 265	72.249 34.299 12.358 1.00 22.96
30	ATOM	836 CB VAL 265	70.910 33.660 11.879 1.00 21.04
	ATOM	837 CG1 VAL 265	70.458 32.600 12.866 1.00 19.48
	ATOM	838 CG2 VAL 265	69.838 34.708 11.698 1.00 18.96
	ATOM	839 C VAL 265	72.718 35.387 11.382 1.00 24.66
	ATOM	840 O VAL 265	73.026 35.103 10.224 1.00 26.03
35	ATOM	841 N ARG 266	72.777 36.628 11.858 1.00 25.11
	ATOM	842 CA ARG 266	73.233 37.729 11.031 1.00 25.60
	ATOM	843 CB ARG 266	72.187 38.819 10.964 1.00 24.09
	ATOM	844 CG ARG 266	71.035 38.427 10.088 1.00 23.37
	ATOM	845 CD ARG 266	69.998 39.492 10.098 1.00 24.80
40	ATOM	846 NE ARG 266	68.961 39.253 9.109 1.00 24.01
	ATOM	847 CZ ARG 266	67.833 39.940 9.069 1.00 23.26
	ATOM	848 NH1 ARG 266	67.613 40.880 9.970 1.00 24.16
	ATOM	849 NH2 ARG 266	66.960 39.733 8.099 1.00 23.31
	ATOM	850 C ARG 266	74.543 38.273 11.543 1.00 28.07
45	ATOM	851 O ARG 266	74.786 39.479 11.517 1.00 29.67
	ATOM	852 N TYR 267	75.367 37.366 12.053 1.00 28.90
	ATOM	853 CA TYR 267	76.679 37.714 12.558 1.00 30.23
	ATOM	854 CB TYR 267	77.223 36.584 13.434 1.00 29.98
	ATOM	855 CG TYR 267	78.699 36.702 13.727 1.00 31.75
50	ATOM	856 CD1 TYR 267	79.179 37.577 14.712 1.00 31.21

	ATOM	857 CE1 TYR 267	80,544 37.705 14.950 1.00 31.29
	ATOM	858 CD2 TYR 267	79.625 35.958 12.994 1.00 31.84
	ATOM	859 CE2 TYR 267	80.986 36.078 13.222 1.00 32.15
	ATOM	860 CZ TYR 267	81.442 36.949 14.197 1.00 32.60
5	ATOM	861 OH TYR 267	82.801 37.052 14.389 1.00 34.13
•	ATOM	862 C TYR 267	77.570 37.900 11.343 1.00 31.17
	ATOM	863 O TYR 267	77.543 37.086 10.426 1.00 30.91
	ATOM	864 N ASP 268	78.361 38.966 11.336 1.00 33.09
	ATOM	865 CA ASP 268	79.252 39.233 10.216 1.00 35.57
10	ATOM	866 CB ASP 268	79.085 40.679 9.747 1.00 39.39
	ATOM	867 CG ASP 268	79.796 40.954 8.432 1.00 42.22
	ATOM	868 OD1 ASP 268	79.426 40.331 7.412 1.00 46.07
	ATOM	869 OD2 ASP 268	80.718 41.798 8.415 1.00 44.30
	ATOM	870 C ASP 268	80.700 38.967 10.620 1.00 35.72
15	ATOM	871 O ASP 268	81.287 39.737 11.384 1.00 34.49
	ATOM	872 N PRO 269	81.295 37.872 10.108 1.00 37.00
	ATOM	873 CD PRO 269	80.712 36.887 9.182 1.00 36.77
	ATOM	874 CA PRO 269	82.679 37.514 10.427 1.00 38.52
	ATOM	875 CB PRO 269	82.905 36.239 9.611 1.00 37.06
20	ATOM	876 CG PRO 269	81.549 35.669 9.453 1.00 36.19
	ATOM	877 C PRO 269	83.656 38.613 10.019 1.00 40.96
	ATOM	878 O PRO 269	84.586 38.929 10.760 1.00 42.23
	ATOM	879 N ALA 270	83.418 39.209 8.854 1.00 41.92
	ATOM	880 CA ALA 270	84.277 40.272 8.342 1.00 42.08
25	ATOM	881 CB ALA 270	83.709 40.838 7.029 1.00 42.64
	ATOM	882 C ALA 270	84.495 41.394 9.355 1.00 41.70
	ATOM	883 O ALA 270	85.632 41.709 9.684 1.00 42.25
	ATOM	884 N SER 271	83.408 41.970 9.865 1.00 41.87
	ATOM	885 CA SER 271	83.495 43.073 10.830 1.00 40.75
30	ATOM	886 CB SER 271	82.454 44.143 10.500 1.00 40.60
	ATOM	887 OG SER 271	81.150 43.590 10.464 1.00 40.31
	ATOM	888 C SER 271	83.344 42.658 12.290 1.00 39.99
	ATOM	889 O SER 271	83.484 43.487 13.194 1.00 38.77
	ATOM	890 N ASP 272	83.042 41.381 12.508 1.00 38.94
35	ATOM	891 CA ASP 272	82.859 40.844 13.845 1.00 37.78
	ATOM	892 CB ASP 272	84.182 40.904 14.625 1.00 38.86
	ATOM	893 CG ASP 272	84.094 40.255 16.000 1.00 41.09
	ATOM	894 OD1 ASP 272	83.342 39.275 16.173 1.00 41.64
	ATOM	895 OD2 ASP 272	84.781 40.734 16.924 1.00 43.84
40	ATOM	896 C ASP 272	81.744 41.634 14.536 1.00 36.92
	ATOM	897 O ASP 272	81.907 42.156 15.648 1.00 37.56
	ATOM	898 N THR 273	80.603 41.723 13.865 1.00 33.65
	ATOM	899 CA THR 273	79.469 42.443 14.425 1.00 31.57
	ATOM	900 CB THR 273	79.246 43.790 13.695 1.00 31.69
45	ATOM	901 OG1 THR 273	79.087 43.557 12.289 1.00 30.71
	ATOM	902 CG2 THR 273	80.426 44.730 13.922 1.00 31.53
	ATOM	903 C THR 273	78.184 41.631 14.310 1.00 30.15
	ATOM	904 O THR 273	78.104 40.697 13.504 1.00 30.10
	ATOM	905 N LEU 274	77.213 41.942 15.164 1.00 27.09
50	ATOM	906 CA LEU 274	75.907 41.303 15.103 1.00 25.94

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75.396 40.936 16.496 1.00 24.47
     ATOM
             907 CB LEU 274
             908 CG LEU 274
                                76.020 39.731 17.206 1.00 23.33
     ATOM
             909 CD1 LEU 274
                                75.436 39.631 18.602 1.00 21.14
     ATOM
                                75.792 38.444 16.427 1.00 20.04
             910 CD2 LEU 274
     ATOM
             911 C LEU 274
                               75.010 42.377 14.500 1.00 26.57
     ATOM
             912 O LEU 274
                               75.339 43.557 14.568 1.00 27.03
     ATOM
             913 N THR 275
                               73.914 41.987 13.865 1.00 26.60
     ATOM
                                73.009 42.966 13.285 1.00 26.48
            914 CA THR 275
     ATOM
             915 CB THR 275
                                72.786 42.717 11.781 1.00 26.52
     ATOM
                                 74.044 42.719 11.097 1.00 28.67
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     ATOM
             916 OG1 THR 275
                                71.919 43.799 11.198 1.00 27.35
            917 CG2 THR 275
     ATOM
                               71.674 42.898 14.014 1.00 26.57
             918 C THR 275
     ATOM
     ATOM
             919 O THR 275
                               71.069 41.825 14.121 1.00 28.50
             920 N LEU 276
                               71.236 44.026 14.564 1.00 25.18
     ATOM
             921 CA LEU 276
                                69.970 44.069 15.276 1.00 24.61
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     ATOM
     ATOM
             922 CB LEU 276
                                70.057 44.987 16.506 1.00 23.61
                                71.199 44.730 17.503 1.00 24.36
     ATOM
            923 CG LEU 276
                                71.039 45.654 18.709 1.00 19.91
     ATOM
            924 CD1 LEU 276
     ATOM
            925 CD2 LEU 276
                                71.225 43.253 17.947 1.00 22.20
20
     ATOM
            926 C LEU 276
                               68.894 44.560 14.322 1.00 25.63
     ATOM
            927 O LEU 276
                               69.100 45.556 13.623 1.00 25.35
            928 N SER 277
                               67.787 43.814 14.249 1.00 25.94
     ATOM
     ATOM
             929 CA SER 277
                               66.634 44.141 13.403 1.00 24.61
     ATOM
             930 CB SER 277
                               65.874 45.335 13.987 1.00 21.96
25
     ATOM
            931 OG SER 277
                                65.368 45.029 15.273 1.00 19.68
                               67.005 44.406 11.946 1.00 25.20
             932 C SER 277
     ATOM
     ATOM
             933 O SER 277
                               66.350 45.199 11.267 1.00 25.21
     ATOM
             934 N GLY 278
                               68.067 43.747 11.489 1.00 27.08
             935 CA GLY 278
                                68.556 43.899 10.127 1.00 29.27
     ATOM
30
     ATOM
             936 C GLY 278
                               69.022 45.297 9.753 1.00 31.57
     ATOM
             937 O GLY 278
                               69.303 45.564 8.591 1.00 31.42
     ATOM
            938 N GLU 279
                               69.159 46.177 10.740 1.00 33.41
             939 CA GLU 279
                                69.558 47.560 10.484 1.00 34.84
     ATOM
             940 CB GLU 279
                                68.345 48.485 10.650 1.00 36.16
     ATOM
             941 CG GLU 279
                                67.843 48.606 12.090 1.00 38.08
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     ATOM
             942 CD GLU 279
                                66.566 49.419 12.206 1.00 41.07
     ATOM
     ATOM
             943 OE1 GLU 279
                                66.475 50.279 13.108 1.00 41.98
                                65.643 49.197 11.399 1.00 43.80
     ATOM
            944 OE2 GLU 279
             945 C GLU 279
                               70.706 48.116 11.326 1.00 34.38
     ATOM
                               71.366 49.057 10.901 1.00 35.60
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     ATOM
             946 O GLU 279
                               70.944 47.565 12.511 1.00 33.43
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             947 N MET 280
             948 CA MET 280
                                72.014 48.085 13.358 1.00 32.27
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                                71.443 48.544 14.702 1.00 31.81
     ATOM
             949 CB MET 280
                                72.471 49.181 15.637 1.00 29.76
     ATOM
             950 CG MET 280
                                71.813 49.482 17.289 1.00 29.63
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     ATOM
             951 SD MET 280
                                70.592 50.735 16.989 1.00 24.91
     ATOM
             952 CE MET 280
                               73.161 47.119 13.603 1.00 32.51
     ATOM
             953 C MET 280
            954 O MET 280
                               72.995 46.117 14.303 1.00 32.78
     ATOM
                               74,321 47.408 13.021 1.00 31.74
             955 N ALA 281
     ATOM
            956 CA ALA 281
                                75.491 46.564 13.231 1.00 32.25
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76.494 46.740 12.108 1.00 30.91
            957 CB ALA 281
     ATOM
                               76.091 47.006 14.563 1.00 33.09
            958 C ALA 281
     ATOM
    ATOM
                               76.261 48.202 14.805 1.00 34.06
            959 O ALA 281
     ATOM
            960 N VAL 282
                               76.358 46.053 15.447 1.00 33.78
            961 CA VAL 282
                                76.913 46.366 16.755 1.00 33.45
    ATOM
                                75.858 46.208 17.885 1.00 34.92
     ATOM
            962 CB VAL 282
                                74.775 47.269 17.744 1.00 34.90
    ATOM
            963 CG1 VAL 282
            964 CG2 VAL 282
                                75.246 44.806 17.860 1.00 34.39
    ATOM
            965 C VAL 282
                               78.119 45.514 17.087 1.00 33.93
    ATOM
            966 O VAL 282
                               78.202 44.347 16.702 1.00 35.11
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     ATOM
                               79.071 46.123 17.777 1.00 33.49
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            967 N LYS 283
    ATOM
            968 CA LYS 283
                               80.285 45.446 18.187 1.00 34.83
    ATOM
            969 CB LYS 283
                               81.446 46.445 18.183 1.00 35.96
            970 CG LYS 283
                               81.726 47.013 16.797 1.00 39.20
    ATOM
            971 CD LYS 283
15
    ATOM
                               82.621 48.245 16.844 1.00 43.38
    ATOM
            972 CE LYS 283
                               83.142 48.611 15.455 1.00 44.17
    ATOM
            973 NZ LYS 283
                               84.077 47.563 14.922 1.00 47.27
    ATOM
            974 C LYS 283
                               80.068 44.832 19.572 1.00 33.94
    ATOM
            975 O LYS 283
                               79.134 45.215 20.290 1.00 33.85
                               80.939 43.895 19.941 1.00 33.63
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    ATOM
            976 N ARG 284
            977 CA ARG 284
                                80.873 43.184 21.217 1.00 34.00
    ATOM
            978 CB ARG 284
                                82.094 42.285 21.381 1.00 34.04
    ATOM
    ATOM
                                82.332 41.369 20.219 1.00 36.31
            979 CG ARG 284
    ATOM
            980 CD ARG 284
                                83.638 40.643 20.354 1.00 37.03
                                83.724 39.576 19.369 1.00 39.27
25
    ATOM
            981 NE ARG 284
    ATOM
            982 CZ ARG 284
                                83.323 38.326 19.583 1.00 40.07
                                82.804 37.973 20.759 1.00 39.78
    ATOM
            983 NH1 ARG 284
            984 NH2 ARG 284
                                83.434 37.428 18.613 1.00 40.16
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            985 C ARG 284
                               80.787 44.101 22.419 1.00 35.16
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30
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            986 O ARG 284
                               79.884 43.977 23.249 1.00 35.87
    ATOM
            987 N GLU 285
                               81.763 44.993 22.530 1.00 35.75
            988 CA GLU 285
                                81.827 45.939 23.632 1.00 36.86
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    ATOM
            989 CB GLU 285
                                83.071 46.818 23.464 1.00 40.47
                                83.202 47.973 24.444 1.00 49.23
    ATOM
            990 CG GLU 285
            991 CD GLU 285
                                83.587 49.284 23.747 1.00 54.22
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    ATOM
            992 OE1 GLU 285
                                84.784 49.657 23.760 1.00 55.37
    ATOM
    ATOM
            993 OE2 GLU 285
                                82.686 49.942 23.176 1.00 56.95
            994 C GLU 285
    ATOM
                               80,552 46,785 23.684 1.00 34.45
    ATOM
            995 O GLU 285
                               79.990 47.007 24.754 1.00 34.47
                               80.046 47.166 22.515 1.00 32.27
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    ATOM
            996 N GLN 286
    ATOM
            997 CA GLN 286
                                78.853 47.991 22.438 1.00 30.35
            998 CB GLN 286
                                78.615 48.472 21.006 1.00 33.34
    ATOM
                                79.632 49.497 20.500 1.00 35.09
    ATOM
            999 CG GLN 286
    ATOM 1000 CD GLN 286
                                79.293 50.023 19.108 1.00 38.42
45
    ATOM 1001 OE1 GLN 286
                                79.161 49.248 18.158 1.00 39.03
    ATOM 1002 NE2 GLN 286
                                79.156 51.339 18.982 1.00 37.82
                               77.605 47.308 22.970 1.00 29.57
    ATOM 1003 C GLN 286
                               76.870 47.891 23.770 1.00 26.96
    ATOM 1004 O GLN 286
    ATOM 1005 N LEU 287
                               77.352 46.080 22.524 1.00 29.50
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    ATOM 1006 CA LEU 287
                                76.164 45.350 22.979 1.00 28.93
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	ATOM	1007 CB LEU 287	75.831 44.182 22.029 1.00 27.14
	ATOM	1008 CG LEU 287	74.474 43.484 22.227 1.00 24.66
	ATOM	1009 CD1 LEU 287	73.316 44.475 22.184 1.00 22.70
	ATOM	1010 CD2 LEU 287	74.297 42.413 21.163 1.00 25.17
5	ATOM	1011 C LEU 287	76.303 44.874 24.433 1.00 28.10
	ATOM	1012 O LEU 287	75.301 44.748 25.155 1.00 28.58
	ATOM	1013 N LYS 288	77.541 44.652 24.868 1.00 27.97
	ATOM	1014 CA LYS 288	77.808 44.218 26.230 1.00 28.55
	ATOM	1015 CB LYS 288	79.270 43.800 26.376 1.00 28.93
10	ATOM	1016 CG LYS 288	79.603 43.254 27.750 1.00 32.46
	ATOM	1017 CD LYS 288	81.015 42.725 27.826 1.00 33.48
	ATOM	1018 CE LYS 288	81.205 41.878 29.071 1.00 35.76
	ATOM	1019 NZ LYS 288	82.525 41.186 29.029 1.00 40.52
	ATOM	1020 C LYS 288	77.497 45.341 27.220 1.00 29.15
15	ATOM	1021 O LYS 288	76.782 45.132 28.207 1.00 31.28
	ATOM	1022 N ASN 289	77.996 46.539 26.933 1.00 28.58
	ATOM	1023 CA ASN 289	77.794 47.692 27.811 1.00 28.40
	ATOM	1024 CB ASN 289	78.815 48.775 27.485 1.00 28.28
	ATOM	1025 CG ASN 289	80.224 48.329 27.770 1.00 31.30
20	ATOM	1026 OD1 ASN 289	80.445 47.442 28.601 1.00 33.02
	ATOM	1027 ND2 ASN 289	81.190 48.928 27.087 1.00 30.49
	ATOM	1028 C ASN 289	76.395 48.278 27.792 1.00 28.33
	ATOM	1029 O ASN 289	76.005 48.977 28.724 1.00 28.36
	ATOM	1030 N GLY 290	75.638 47.977 26.740 1.00 26.71
25	ATOM	1031 CA GLY 290	74.286 48.487 26.606 1.00 23.27
	ATOM	1032 C GLY 290	73.233 47.852 27.484 1.00 22.93
	ATOM	1033 O GLY 290	72.063 48.219 27.399 1.00 23.84
	ATOM	1034 N GLY 291	73.620 46.905 28.330 1.00 21.30
	ATOM	1035 CA GLY 291	72.637 46.290 29.199 1.00 20.38
30	ATOM	1036 C GLY 291	72.653 44.778 29.200 1.00 20.05
	ATOM	1037 O GLY 291	72.190 44.165 30.147 1.00 21.91
	ATOM	1038 N LEU 292	73.211 44.173 28.160 1.00 21.36
	ATOM	1039 CA LEU 292	73.248 42.717 28.062 1.00 21.51
	ATOM	1040 CB LEU 292	73.319 42.280 26.593 1.00 18.52
35	ATOM	1041 CG LEU 292	72.019 42.506 25.815 1.00 17.07
	ATOM	1042 CD1 LEU 292	72.103 41.818 24.479 1.00 18.09
	ATOM	1043 CD2 LEU 292	70.844 41.947 26.599 1.00 16.35
	ATOM	1044 C LEU 292	74.347 42.046 28.872 1.00 22.17
40	ATOM	1045 O LEU 292	74.176 40.923 29.352 1.00 21.91
40	ATOM	1046 N GLY 293	75.479 42.724 29.011 1.00 23.76 76.588 42.169 29.760 1.00 23.92
	ATOM ATOM	1047 CA GLY 293 1048 C GLY 293	76.388 42.169 29.760 1.00 23.92 77.134 40.926 29.091 1.00 25.09
		1048 C GLY 293 1049 O GLY 293	77.362 40.919 27.883 1.00 26.51
	ATOM	1049 O GL1 293 1050 N VAL 294	77.332 39.866 29.867 1.00 26.08
45	ATOM ATOM	1050 N VAL 294 1051 CA VAL 294	77.854 38.618 29.329 1.00 26.34
43	ATOM	1051 CA VAL 294	78.263 37.636 30.443 1.00 26.97
	ATOM		79.440 38.199 31.209 1.00 28.20
	ATOM		77.099 37.371 31.384 1.00 25.56
	ATOM	1055 C VAL 294	76.891 37.937 28.360 1.00 26.41
50	ATOM	1056 O VAL 294	77.315 37.097 27.568 1.00 27.65
50	AION	1000 O VAL 204	77.515 57.077 27.500 1.00 27.05

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	ATOM	1057 N VAL 295	75.608 38.304 28.408 1.00 26.09
	ATOM	1058 CA VAL 295	74.606 37.740 27.499 1.00 26.65
	ATOM	1059 CB VAL 295	73.186 38.312 27.777 1.00 28.39
	ATOM	1060 CG1 VAL 295	72.164 37.740 26.782 1.00 26.69
5	ATOM	1061 CG2 VAL 295	72.763 38.005 29.206 1.00 26.23
	ATOM	1062 C VAL 295	75.035 38.089 26.069 1.00 25.83
	ATOM	1063 O VAL 295	74.903 37.286 25.151 1.00 27.12
	ATOM	1064 N SER 296	75.609 39.275 25.908 1.00 24.95
	ATOM	1065 CA SER 296	76.097 39.725 24.619 1.00 26.17
10	ATOM	1066 CB SER 296	76.665 41.132 24.742 1.00 25.82
	ATOM	1067 OG SER 296	77.253 41.554 23.525 1.00 26.64
	ATOM	1068 C SER 296	77.196 38.783 24.142 1.00 28.63
	ATOM	1069 O SER 296	77.241 38.420 22.963 1.00 29.19
	ATOM	1070 N ASP 297	78.118 38.443 25.046 1.00 29.69
15	ATOM	1071 CA ASP 297	79.211 37.531 24.731 1.00 28.96
15	ATOM	1071 CA ASI 297	80.058 37.234 25.973 1.00 31.82
	ATOM	1072 CB ASP 297	80.768 38.454 26.506 1.00 35.23
	ATOM	1074 OD1 ASP 297	80.958 39.429 25.743 1.00 35.71
	ATOM	1074 ODI ASI 297 1075 OD2 ASP 297	81.140 38.430 27.698 1.00 37.68
20	ATOM	1075 OD2 ASI 257 1076 C ASP 297	78.605 36.227 24.247 1.00 27.63
20	ATOM	1070 C ASP 297	79.048 35.666 23.248 1.00 29.88
	ATOM	1077 O ASF 297 1078 N ALA 298	77.581 35.762 24.952 1.00 25.15
	ATOM	1079 CA ALA 298	76.909 34.527 24.592 1.00 24.49
	ATOM	1079 CA ALA 298 1080 CB ALA 298	75.811 34.224 25.594 1.00 21.91
25	ATOM	1080 CB ALA 298	76.343 34.569 23.158 1.00 24.93
23	ATOM	1081 C ALA 298	76.589 33.654 22.357 1.00 24.83
	ATOM	1082 O ALA 298 1083 N ILE 299	75.632 35.647 22.814 1.00 24.70
	ATOM	1084 CA ILE 299	75.041 35.756 21.480 1.00 22.49
	ATOM	1085 CB ILE 299	74.057 36.950 21.351 1.00 21.96
30	ATOM	1086 CG2 ILE 299	73.338 36.876 20.005 1.00 19.17
30	ATOM	1080 CG2 ILE 299	72.994 36.876 22.459 1.00 21.16
	ATOM	1087 CGI ILE 299	72.363 38.228 22.853 1.00 22.04
	ATOM	1088 CDI ILE 299	76.127 35.829 20.428 1.00 22.33
	ATOM	1089 C ILE 299 1090 O ILE 299	75.995 35.234 19.367 1.00 24.80
25		1090 O ILE 299 1091 N PHE 300	77.209 36.538 20.724 1.00 21.92
35	ATOM	1091 N PHE 300 1092 CA PHE 300	78.322 36.641 19.785 1.00 23.08
	ATOM	1092 CA PHE 300 1093 CB PHE 300	79.385 37.636 20.278 1.00 24.08
	ATOM ATOM		79.249 39.017 19.686 1.00 24.18
			78.494 39.991 20.325 1.00 24.18
40	ATOM	1095 CD1 PHE 300	79.857 39.331 18.471 1.00 23.76
40	ATOM	1096 CD2 PHE 300	78.347 41.253 19.770 1.00 22.38
	ATOM	1097 CE1 PHE 300	
	ATOM	1098 CE2 PHE 300	79.715 40.596 17.904 1.00 23.21
	ATOM	1099 CZ PHE 300	78.957 41.558 18.554 1.00 22.46
15	ATOM	1100 C PHE 300	78.948 35.274 19.561 1.00 23.06
45	ATOM	1101 O PHE 300	79.264 34.913 18.426 1.00 23.97
	ATOM	1102 N GLU 301	79.113 34.506 20.636 1.00 23.75
	ATOM	1103 CA GLU 301	79.694 33.169 20.525 1.00 24.16
	ATOM	1104 CB GLU 301	79.884 32.545 21.902 1.00 23.03
	ATOM	1105 C GLU 301	78.776 32.302 19.672 1.00 23.62
50	ATOM	1106 O GLU 301	79.240 31.591 18.777 1.00 25.11

	ATOM	1107 N LEU 302	77.472 32.394 19.926 1.00 23.12
	ATOM	1108 CA LEU 302	76.495 31.624 19.166 1.00 23.56
	ATOM	1109 CB LEU 302	75.082 31.865 19.701 1.00 21.75
_	ATOM	1110 CG LEU 302	73.953 31.120 18.979 1.00 22.61
5	ATOM	1111 CD1 LEU 302	74.084 29.612 19.193 1.00 22.31
	ATOM	1112 CD2 LEU 302	72.611 31.604 19.485 1.00 19.27
	ATOM	1113 C LEU 302	76.588 32.011 17.687 1.00 24.41 76.670 31.140 16.814 1.00 24.63
	ATOM	1114 O LEU 302	76.651 33.316 17.425 1.00 25.69
	ATOM	1115 N GLY 303	76.746 33.816 17.423 1.00 25.87
10	ATOM	1116 CA GLY 303	77.975 33.288 15.338 1.00 28.63
	ATOM	1117 C GLY 303	
	ATOM	1118 O GLY 303	77.893 32.895 14.170 1.00 28.30 79.116 33.279 16.023 1.00 29.53
	ATOM	1119 N LYS 304	
	ATOM	1120 CA LYS 304	80.360 32.791 15.437 1.00 31.18 81.529 32.931 16.418 1.00 34.79
15	ATOM	1121 CB LYS 304	81.529 32.931 16.418 1.00 34.79 82.157 34.307 16.506 1.00 40.28
	ATOM	1122 CG LYS 304	83,441 34.262 17.332 1.00 44.37
	ATOM	1123 CD LYS 304 1124 CE LYS 304	83,174 33,814 18,775 1.00 47.63
	ATOM	1124 CE LYS 304 1125 NZ LYS 304	82.459 34.847 19.592 1.00 48.83
20	ATOM	1125 NZ L13 304 1126 C LYS 304	80.245 31.328 15.042 1.00 30.87
20	ATOM ATOM	1126 C LTS 304 1127 O LYS 304	80.632 30.944 13.932 1.00 29.53
	ATOM	1127 O E13 304 1128 N SER 305	79.720 30.518 15.961 1.00 30.46
	ATOM	1129 CA SER 305	79.566 29.086 15.731 1.00 31.09
	ATOM	1130 CB SER 305	79,243 28.370 17.041 1.00 29.83
25	ATOM	1131 OG SER 305	77.990 28.783 17.550 1.00 34.66
23	ATOM	1132 C SER 305	78.532 28.732 14.653 1.00 31.06
	ATOM	1133 O SER 305	78.745 27.799 13.872 1.00 31.84
	ATOM	1134 N LEU 306	77.436 29.491 14.594 1.00 29.43
	ATOM	1135 CA LEU 306	76.378 29.258 13.611 1.00 28.39
30	ATOM	1136 CB LEU 306	75.121 30.055 13.962 1.00 26.05
	ATOM	1137 CG LEU 306	74.306 29.573 15.157 1.00 26.33
	ATOM	1138 CD1 LEU 306	73.061 30.430 15.285 1.00 26.22
	ATOM	1139 CD2 LEU 306	73.924 28.110 14.985 1.00 25.86
	ATOM	1140 C LEU 306	76.754 29.529 12.157 1.00 28.66
35	ATOM	1141 O LEU 306	76.116 29.001 11.253 1.00 28.58
	ATOM	1142 N SER 307	77.786 30.338 11.931 1.00 29.72
	ATOM	1143 CA SER 307	78.224 30.667 10.577 1.00 31.19
	ATOM	1144 CB SER 307	79.466 31.556 10.617 1.00 30.15
	ATOM	1145 OG SER 307	79.226 32.710 11.396 1.00 35.19
40	ATOM	1146 C SER 307	78.531 29.412 9.777 1.00 32.75
	ATOM	1147 O SER 307	78.110 29.283 8.621 1.00 33.09
	ATOM	1148 N ALA 308	79.248 28.482 10.407 1.00 33.36
	ATOM	1149 CA ALA 308	79.626 27.223 9.769 1.00 34.50
	ATOM	1150 CB ALA 308	80.636 26.473 10.637 1.00 33.55
45	ATOM	1151 C ALA 308	78.417 26.328 9.466 1.00 35.00
	ATOM	1152 O ALA 308	78.469 25.501 8.550 1.00 37.10
	ATOM	1153 N PHE 309	77.335 26.496 10.226 1.00 32.76
	ATOM	1154 CA PHE 309	76.134 25.698 10.028 1.00 31.73
	ATOM	1155 CB PHE 309	75.214 25.818 11.232 1.00 30.04
50	ATOM	1156 CG PHE 309	75.705 25.091 12.438 1.00 31.19

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74.973 24.048 12.975 1.00 31.61
    ATOM 1157 CD1 PHE 309
                                76.884 25.459 13.054 1.00 31.92
    ATOM 1158 CD2 PHE 309
                                75.400 23.391 14.110 1.00 31.22
    ATOM 1159 CE1 PHE 309
    ATOM 1160 CE2 PHE 309
                               77.320 24.807 14.194 1.00 31.01
    ATOM 1161 CZ PHE 309
                               76.577 23.771 14.720 1.00 30.47
                              75.364 26.050 8.753 1.00 31.53
    ATOM 1162 C PHE 309
                               74.516 25.269 8.310 1.00 31.28
    ATOM 1163 O PHE 309
    ATOM 1164 N ASN 310
                               75.661 27.220 8.181 1.00 31.12
                               75.020 27.711 6.957 1.00 30.34
    ATOM 1165 CA ASN 310
10
    ATOM 1166 CB ASN 310
                               75.636 27.036 5.719 1.00 31.63
                               73.511 27.492 7.003 1.00 29.40
    ATOM 1167 C ASN 310
    ATOM 1168 O ASN 310
                               72.939 26.791 6.156 1.00 29.15
    ATOM 1169 N LEU 311
                               72.875 28.055 8.026 1.00 27.60
    ATOM 1170 CA LEU 311
                               71.435 27.907 8.205 1.00 28.23
                               71.021 28.313 9.621 1.00 27.41
    ATOM 1171 CB LEU 311
15
    ATOM 1172 CG LEU 311
                               71.603 27.558 10.822 1.00 26.80
    ATOM 1173 CD1 LEU 311
                                70.949 28.078 12.112 1.00 25.05
    ATOM 1174 CD2 LEU 311 71.360 26.062 10.662 1.00 24.72
                               70.628 28.719 7.192 1.00 29.01
    ATOM 1175 C LEU 311
    ATOM 1176 O LEU 311
                               71.040 29.808 6.782 1.00 30.66
20
    ATOM 1177 N ASP 312
                              69.503 28.168 6.748 1.00 26.30
                               68.675 28.894 5.817 1.00 25.13
    ATOM 1178 CA ASP 312
                               68.391 28.067 4.539 1.00 23.90
    ATOM 1179 CB ASP 312
    ATOM 1180 CG ASP 312
                               67.438 26.890 4.754 1.00 21.34
25
    ATOM 1181 OD1 ASP 312
                                66.959 26.631 5.868 1.00 22.47
    ATOM 1182 OD2 ASP 312
                                67.154 26.206 3.758 1.00 22.18
    ATOM 1183 C ASP 312
                              67.419 29.379 6.542 1.00 24.49
    ATOM 1184 O ASP 312
                              67.221 29.056 7.725 1.00 24.01
    ATOM 1185 N ASP 313
                               66.587 30.153 5.845 1.00 23.40
    ATOM 1186 CA ASP 313
                               65.363 30.697 6.421 1.00 22.63
30
                               64.557 31.486 5.385 1.00 24.99
    ATOM 1187 CB ASP 313
                               65.224 32.799 4.994 1.00 28.02
    ATOM 1188 CG ASP 313
                                66.036 33.334 5.778 1.00 30.34
    ATOM 1189 OD1 ASP 313
    ATOM 1190 OD2 ASP 313
                                64.936 33.306 3.897 1.00 30.41
                              64.480 29.650 7.053 1.00 21.47
    ATOM 1191 C ASP 313
35
                              63.853 29.917 8.082 1.00 21.76
    ATOM 1192 O ASP 313
                               64.407 28.474 6.435 1.00 19.16
    ATOM 1193 N THR 314
                                63.580 27.386 6.966 1.00 18.79
    ATOM 1194 CA THR 314
    ATOM 1195 CB THR 314
                               63.398 26.240 5.913 1.00 19.68
    ATOM 1196 OG1 THR 314
                                62.743 26.758 4.747 1.00 20.56
40
    ATOM 1197 CG2 THR 314
                                62.558 25.112 6.482 1.00 18.84
                               64.133 26.818 8.293 1.00 15.38
    ATOM 1198 C THR 314
    ATOM 1199 O THR 314
                               63.383 26.538 9.223 1.00 14.08
                               65.445 26.656 8.376 1.00 15.16
    ATOM 1200 N GLU 315
45
    ATOM 1201 CA GLU 315
                                66.051 26.126 9.593 1.00 16.78
    ATOM 1202 CB GLU 315
                                67.513 25.785 9.340 1.00 14.29
    ATOM 1203 CG GLU 315
                                67.611 24.483 8.579 1.00 15.13
    ATOM 1204 CD GLU 315
                                68.910 24.291 7.872 1.00 15.90
                                69.625 25.285 7.639 1.00 19.80
    ATOM 1205 OE1 GLU 315
    ATOM 1206 OE2 GLU 315
                                69,211 23.129 7.527 1.00 19.34
50
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	ATOM	1207 C GLU 315	65.872 27.119 10.736 1.00 17.27
	ATOM	1208 O GLU 315	65.457 26.742 11.836 1.00 17.46
	ATOM	1209 N VAL 316	66.081 28.399 10.440 1.00 17.12
	ATOM	1210 CA VAL 316	65.897 29.441 11.446 1.00 16.92
5	ATOM	1211 CB VAL 316	66.336 30.828 10.918 1.00 15.89
	ATOM	1212 CG1 VAL 316	66.062 31.921 11.962 1.00 14.60
	ATOM	1213 CG2 VAL 316	67.811 30.785 10.579 1.00 15.95
	ATOM	1214 C VAL 316	64.430 29.472 11.869 1.00 17.32
	ATOM	1215 O VAL 316	64.131 29.582 13.055 1.00 18.11
10	ATOM	1216 N ALA 317	63.515 29.324 10.905 1.00 17.42
	ATOM	1217 CA ALA 317	62.076 29.342 11.195 1.00 16.21
	ATOM	1218 CB ALA 317	61.262 29.321 9.910 1.00 14.63
	ATOM	1219 C ALA 317	61.656 28.181 12.079 1.00 16.84
	ATOM	1220 O ALA 317	60.904 28.359 13.036 1.00 16.08
15	ATOM	1221 N LEU 318	62.146 26.990 11.759 1.00 17.27
	ATOM	1222 CA LEU 318	61.783 25.804 12.526 1.00 17.88
	ATOM	1223 CB LEU 318	62.141 24.525 11.748 1.00 17.58
	ATOM	1224 CG LEU 318	61.331 24.333 10.439 1.00 16.87
	ATOM	1225 CD1 LEU 318	61.837 23.155 9.658 1.00 15.79
20	ATOM	1226 CD2 LEU 318	59.860 24.149 10.728 1.00 14.08
	ATOM	1227 C LEU 318	62.394 25.852 13.932 1.00 18.20
	ATOM	1228 O LEU 318	61.733 25.495 14.910 1.00 18.71
	ATOM	1229 N LEU 319	63.614 26.380 14.034 1.00 17.73
	ATOM	1230 CA LEU 319	64.288 26.531 15.321 1.00 16.57
25	ATOM	1231 CB LEU 319	65.689 27.105 15.107 1.00 18.81
	ATOM	1232 CG LEU 319	66.733 27.223 16.224 1.00 21.77
	ATOM	1233 CD1 LEU 319	66.767 25.994 17.117 1.00 23.03
	ATOM	1234 CD2 LEU 319	68.076 27.421 15.554 1.00 20.86
	ATOM	1235 C LEU 319	63.433 27.471 16.160 1.00 16.07
30	ATOM	1236 O LEU 319	63.134 27.183 17.319 1.00 16.40
	ATOM	1237 N GLN 320	62.948 28.546 15.545 1.00 13.91
	ATOM	1238 CA GLN 320	62.101 29.490 16.253 1.00 13.86
	ATOM	1239 CB GLN 320	61.782 30.697 15.373 1.00 13.26
	ATOM	1240 CG GLN 320	62.994 31.553 15.080 1.00 12.17
35	ATOM	1241 CD GLN 320	62.691 32.802 14.253 1.00 13.98
	ATOM	1242 OE1 GLN 320	63.597 33.568 13.950 1.00 15.61
	ATOM	1243 NE2 GLN 320	61.436 32.993 13.862 1.00 13.85
	ATOM	1244 C GLN 320	60.813 28.832 16.746 1.00 14.52
	ATOM	1245 O GLN 320	60.367 29.087 17.864 1.00 15.12
40	ATOM	1246 N ALA 321	60.211 27.982 15.924 1.00 14.21
	ATOM	1247 CA ALA 321	58.976 27.298 16.309 1.00 15.04
	ATOM	1248 CB ALA 321	58.408 26.519 15.115 1.00 13.84
	ATOM	1249 C ALA 321	59.217 26.349 17.487 1.00 15.98
	ATOM	1250 O ALA 321	58.358 26.197 18.355 1.00 15.12
45	ATOM	1251 N VAL 322	60.373 25.687 17.488 1.00 16.63
	ATOM	1252 CA VAL 322	60.720 24.757 18.557 1.00 18.74
	ATOM	1253 CB VAL 322	62.012 23.943 18.231 1.00 19.42
	ATOM	1254 CG1 VAL 322	62.493 23.154 19.455 1.00 19.45
	ATOM	1255 CG2 VAL 322	61.745 22.986 17.083 1.00 19.05
50	ATOM	1256 C VAL 322	60.910 25.556 19.833 1.00 18.42

	ATOM	1257 O VAL 322	60.421 25.164 20.886 1.00 19.46
	ATOM	1258 N LEU 323	61.607 26.685 19.735 1.00 18.65
	ATOM	1259 CA LEU 323	61.836 27.543 20.894 1.00 18.49
	ATOM	1260 CB LEU 323	62.710 28.740 20.508 1.00 18.36
5	ATOM	1261 CG LEU 323	64.179 28.449 20.186 1.00 18.13
	ATOM	1262 CD1 LEU 323	64.829 29.669 19.585 1.00 17.37
	ATOM	1263 CD2 LEU 323	64.923 27.999 21.447 1.00 17.27
	ATOM	1264 C LEU 323	60.499 28.029 21.454 1.00 18.38
	ATOM	1265 O LEU 323	60.275 28.008 22.663 1.00 18.81
10	ATOM	1266 N LEU 324	59.595 28.406 20.557 1.00 18.67
	ATOM	1267 CA LEU 324	58.275 28.897 20.924 1.00 19.02
	ATOM	1268 CB LEU 324	57.564 29.467 19.685 1.00 17.78
	ATOM	1269 CG LEU 324	56.095 29.891 19.838 1.00 17.59
	ATOM	1270 CD1 LEU 324	55.983 31.123 20.709 1.00 18.15
15	ATOM	1271 CD2 LEU 324	55.489 30.180 18.476 1.00 16.43
	ATOM	1272 C LEU 324	57.354 27.884 21.610 1.00 19.62
	ATOM	1273 O LEU 324	56.735 28.185 22.633 1.00 19.40
	ATOM	1274 N MET 325	57.224 26.701 21.029 1.00 21.14
20	ATOM	1275 CA MET 325	56.330 25.680 21.585 1.00 24.06
20	ATOM	1276 CB MET 325	55.857 24.738 20.473 1.00 24.68 55.169 25.444 19.303 1.00 24.49
	ATOM	1277 CG MET 325 1278 SD MET 325	53.759 26.457 19.820 1.00 26.18
	ATOM ATOM	1278 SD MET 325	52.609 25.252 20.373 1.00 24.03
	ATOM	1279 CE MET 325	56.996 24.887 22.705 1.00 24.05
25	ATOM	1281 O MET 325	57.021 23.664 22.693 1.00 25.68
23	ATOM	1281 O MET 323 1282 N SER 326	57.555 25.593 23.671 1.00 29.34
	ATOM	1283 CA SER 326	58.232 24.938 24.774 1.00 32.40
	ATOM	1284 CB SER 326	59.512 25.701 25.112 1.00 32.12
	ATOM	1285 OG SER 326	60.127 25.173 26.272 1.00 36.86
30	ATOM	1286 C SER 326	57.317 24.831 25.996 1.00 34.04
	ATOM	1287 O SER 326	56.532 25.741 26.280 1.00 33.24
	ATOM	1288 N THR 327	57.366 23.687 26.674 1.00 35.62
	ATOM	1289 CA THR 327	56.560 23.486 27.867 1.00 36.88
	ATOM	1290 CB THR 327	55.938 22.085 27.907 1.00 36.58
35	ATOM	1291 OG1 THR 327	56.953 21.094 27.714 1.00 38.58
	ATOM	1292 CG2 THR 327	54.883 21.938 26.826 1.00 37.73
	ATOM	1293 C THR 327	57.378 23.733 29.135 1.00 38.77
	ATOM	1294 O THR 327	56.921 23.438 30.240 1.00 39.53
	ATOM	1295 N ASP 328	58.593 24.260 28.972 1.00 41.25
40	ATOM	1296 CA ASP 328	59.473 24.573 30.099 1.00 43.20
	ATOM	1297 CB ASP 328	60.940 24.698 29.655 1.00 46.47
	ATOM	1298 CG ASP 328	61.618 23.346 29.439 1.00 51.94
	ATOM	1299' OD1 ASP 328	62.547 23.278 28.601 1.00 55.43
	ATOM	1300 OD2 ASP 328	61.251 22.354 30.111 1.00 54.77
45	ATOM	1301 C ASP 328	59.001 25.905 30.653 1.00 43.79
	ATOM	1302 O ASP 328	59.755 26.877 30.709 1.00 45.91
	ATOM	1303 N ARG 329	57.724 25.967 30.995 1.00 43.55 57.143 27.178 31.542 1.00 43.04
	ATOM	1304 CA ARG 329 1305 CB ARG 329	56.398 27.997 30.482 1.00 43.87
50	ATOM ATOM	1305 CB ARG 329 1306 CG ARG 329	57.258 28.740 29.504 1.00 40.87
<i>5</i> 0	ATUM	1300 CG ARG 329	31.230 20.140 27.304 1.00 40.87

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	ATOM	1307 CD ARG 329	57.545 27.886 28.314 1.00 39.52
	ATOM	1308 NE ARG 329	58.301 28.643 27.341 1.00 38.90
	ATOM	1309 CZ ARG 329	59.624 28.708 27.313 1.00 40.59
	ATOM	1310 NH1 ARG 329	60.359 28.052 28.196 1.00 42.41
5	ATOM	1311 NH2 ARG 329	60.210 29.466 26.413 1.00 41.87
•	ATOM	1312 C ARG 329	56.152 26.817 32.609 1.00 43.00
	ATOM	1313 O ARG 329	55,600 25.716 32.628 1.00 43.66
	ATOM	1314 N SER 330	55.886 27.797 33.456 1.00 41.58
	ATOM	1315 CA SER 330	54.953 27.641 34.538 1.00 40.11
10	ATOM	1316 CB SER 330	55.491 28.362 35.777 1.00 40.38
- 0	ATOM	1317 C SER 330	53.602 28.223 34.103 1.00 38.99
	ATOM	1318 O SER 330	53.553 29.172 33.320 1.00 39.22
	ATOM	1319 N GLY 331	52.517 27.581 34.529 1.00 37.52
	ATOM	1320 CA GLY 331	51.176 28.063 34.232 1.00 35.64
15	ATOM	1321 C GLY 331	50.493 27.782 32.906 1.00 35.14
	ATOM	1322 O GLY 331	49.439 28.363 32.640 1.00 34.48
	ATOM	1323 N LEU 332	51.059 26.925 32.066 1.00 34.54
	ATOM	1324 CA LEU 332	50,424 26,637 30,780 1.00 34,59
	ATOM	1325 CB LEU 332	51.394 25.942 29.828 1.00 33.09
20	ATOM	1326 CG LEU 332	52.532 26.765 29.236 1.00 32.72
	ATOM	1327 CD1 LEU 332	53.473 25.834 28.497 1.00 30.29
	ATOM	1328 CD2 LEU 332	51.987 27.844 28.313 1.00 29.20
	ATOM	1329 C LEU 332	49.191 25.763 30.969 1.00 35.14
	ATOM	1330 O LEU 332	49.178 24.874 31.811 1.00 35.96
25	ATOM	1331 N LEU 333	48.153 26.076 30.204 1.00 35.65
	ATOM	1332 CA LEU 333	46.898 25.345 30.215 1.00 37.97
	ATOM	1333 CB LEU 333	45.743 26.271 29.796 1.00 40.71
	ATOM	1334 CG LEU 333	45.389 27.483 30.670 1.00 43.46
	ATOM [·]	1335 CD1 LEU 333	44.713 28.620 29.882 1.00 42.72
30	ATOM	1336 CD2 LEU 333	44.487 27.021 31.806 1.00 45.25
	ATOM	1337 C LEU 333	46.952 24.115 29.300 1.00 37.78
	ATOM	1338 O LEU 333	46.695 22.991 29.720 1.00 37.65
	ATOM	1339 N CYA 334	47.361 24.323 28.060 1.00 38.65
	ATOM	1340 CA CYA 334	47.413 23.249 27.073 1.00 40.91
35	ATOM	1341 CB CYA 334	46.936 23.788 25.721 1.00 47.35
	ATOM	1342 SG CYA 334	45.406 24.693 25.867 1.00 52.24
	ATOM	1343 AS CYA 334	44.066 22.890 25.562 1.00 70.72
	ATOM	1344 C CYA 334	48.778 22.588 26.901 1.00 39.85
	ATOM	1345 O CYA 334	49.287 22.473 25.775 1.00 39.54
40	ATOM	1346 N VAL 335	49.329 22.078 27.997 1.00 37.67
	ATOM	1347 CA VAL 335	50.641 21.432 27.967 1.00 36.07
	ATOM	1348 CB VAL 335	51.019 20.905 29.384 1.00 33.70
	ATOM	1349 CG1 VAL 335	52.434 20.332 29.401 1.00 33.70
	ATOM	1350 CG2 VAL 335	50.913 22.028 30.387 1.00 31.84
45	ATOM	1351 C VAL 335	50.734 20.334 26.885 1.00 36.09
	ATOM	1352 O VAL 335	51.662 20.335 26.064 1.00 34.41
	ATOM	1353 N ASP 336	49.747 19.444 26.833 1.00 35.95
	ATOM	1354 CA ASP 336	49.748 18.372 25.844 1.00 36.34
_	ATOM		48.591 17.394 26.091 1.00 41.36
50	ATOM	1356 CG ASP 336	48.613 16.206 25.129 1.00 46.23

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47.615 16.021 24.392 1.00 49.55
     ATOM 1357 OD1 ASP 336
                                49.639 15.470 25.097 1.00 48.07
     ATOM 1358 OD2 ASP 336
                               49.727 18.846 24.390 1.00 33.05
     ATOM 1359 C ASP 336
                               50.527 18.377 23.573 1.00 32.33
     ATOM 1360 O ASP 336
                               48.794 19.743 24.076 1.00 29.57
     ATOM 1361 N LYS 337
                               48.661 20.286 22.723 1.00 27.76
     ATOM 1362 CA LYS 337
                               47.520 21.313 22.689 1.00 27.09
     ATOM 1363 CB LYS 337
                               49.988 20.941 22.286 1.00 27.64
     ATOM 1364 C LYS 337
     ATOM 1365 O LYS 337
                               50.472 20.713 21.173 1.00 26.09
     ATOM 1366 N ILE 338
                              50.597 21.688 23.208 1.00 25.90
10
     ATOM 1367 CA ILE 338
                               51.852 22.394 22.971 1.00 24.21
     ATOM 1368 CB ILE 338
                               52.128 23.391 24.122 1.00 23.30
                               53.500 24.048 23.958 1.00 21.75
     ATOM 1369 CG2 ILE 338
     ATOM 1370 CG1 ILE 338
                               51.014 24.448 24.155 1.00 21.19
     ATOM 1371 CD1 ILE 338
                                51.055 25.393 25.361 1.00 21.39
15
                              53.041 21.451 22.782 1.00 25.55
     ATOM 1372 C ILE 338
     ATOM 1373 O ILE 338
                              53.861 21.640 21.875 1.00 24.74
     ATOM 1374 N GLU 339
                               53.124 20.421 23.622 1.00 27.43
     ATOM 1375 CA GLU 339
                                54.220 19.448 23.536 1.00 27.60
20
     ATOM 1376 CB GLU 339
                                54.201 18.512 24.755 1.00 27.21
     ATOM 1377 C GLU 339
                               54.112 18.650 22.236 1.00 26.85
                               55.119 18.385 21.581 1.00 26.71
     ATOM 1378 O GLU 339
     ATOM 1379 N LYS 340
                               52.888 18.276 21.872 1.00 27.04
     ATOM 1380 CA LYS 340
                                52.663 17.515 20.654 1.00 28.19
                               51.210 17.008 20.609 1.00 28.67
25
     ATOM 1381 CB LYS 340
                               53.002 18.402 19.439 1.00 27.96
     ATOM 1382 C LYS 340
                               53.558 17.934 18.436 1.00 27.48
     ATOM 1383 O LYS 340
     ATOM 1384 N SER 341
                               52.746 19.700 19.567 1.00 28.32
     ATOM 1385 CA SER 341
                                53.058 20.662 18.514 1.00 28.02
     ATOM 1386 CB SER 341
                                52.457 22.022 18.867 1.00 31.25
30
     ATOM 1387 OG SER 341
                                52.880 23.029 17.965 1.00 37.69
                               54.578 20.773 18.350 1.00 26.01
     ATOM 1388 C SER 341
                               55.096 20.717 17.234 1.00 25.06
     ATOM 1389 O SER 341
                               55.297 20.899 19.462 1.00 25.71
     ATOM 1390 N GLN 342
     ATOM 1391 CA GLN 342
                                56.750 20.993 19.398 1.00 26.39
35
                                57.356 21.254 20.777 1.00 24.17
     ATOM 1392 CB GLN 342
                                58.834 21.590 20.703 1.00 25.09
     ATOM 1393 CG GLN 342
     ATOM 1394 CD GLN 342
                                59.476 21.677 22.057 1.00 26.93
                                59.479 20.704 22.810 1.00 27.77
     ATOM 1395 OE1 GLN 342
40
     ATOM 1396 NE2 GLN 342
                                60.022 22.839 22.386 1.00 24.61
     ATOM 1397 C GLN 342
                               57.354 19.715 18.806 1.00 25.69
     ATOM 1398 O GLN 342
                               58.356 19.771 18.075 1.00 24.99
     ATOM 1399 N GLU 343
                               56.753 18.569 19.127 1.00 25.00
                                57.222 17.280 18.610 1.00 25.34
     ATOM 1400 CA GLU 343
45
     ATOM 1401 CB GLU 343
                                56.411 16.118 19.245 1.00 25.90
     ATOM 1402 C GLU 343
                               57.089 17.276 17.076 1.00 24.32
     ATOM 1403 O GLU 343
                               58.021 16.891 16.365 1.00 23.99
                               55,961 17.789 16.587 1.00 23.56
     ATOM 1404 N ALA 344
                                55.701 17.875 15.153 1.00 22.85
     ATOM 1405 CA ALA 344
                                54.320 18.451 14.917 1.00 22.64
50
     ATOM 1406 CB ALA 344
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	ATOM	1407 C ALA 344	56.768 18.743 14.489 1.00 22.77
	ATOM	1408 O ALA 344	57.355 18.360 13.477 1.00 22.08
	ATOM	1409 N TYR 345	57.057 19.893 15.092 1.00 21.89
	ATOM	1410 CA TYR 345	58.075 20.792 14.550 1.00 21.18
5	ATOM	1411 CB TYR 345	58.108 22.119 15.313 1.00 20.27
	ATOM	1412 CG TYR 345	57.048 23.078 14.856 1.00 17.45
	ATOM	1413 CD1 TYR 345	56.001 23.431 15.698 1.00 17.99
	ATOM	1414 CE1 TYR 345	54.992 24.253 15.270 1.00 19.97
	ATOM	1415 CD2 TYR 345	57.063 23.589 13.562 1.00 19.11
10	ATOM	1416 CE2 TYR 345	56.055 24.424 13.116 1.00 19.14
10	ATOM	1417 CZ TYR 345	55.017 24.749 13.972 1.00 20.78
	ATOM	1418 OH TYR 345	53.983 25.539 13.530 1.00 20.70
	ATOM	1419 C TYR 345	59.454 20.167 14.583 1.00 20.96
	ATOM	1420 O TYR 345	60.221 20.314 13.632 1.00 22.29
15	ATOM	1421 N LEU 346	59.778 19.480 15.677 1.00 20.82
13	ATOM	1422 CA LEU 346	61.079 18.838 15.817 1.00 20.18
	ATOM	1423 CB LEU 346	61.216 18.203 17.205 1.00 21.04
	ATOM	1424 CG LEU 346	61.606 19.158 18.335 1.00 21.25
	ATOM	1425 CD1 LEU 346	61.226 18.595 19.685 1.00 20.95
20	ATOM	1426 CD2 LEU 346	63.099 19.438 18.267 1.00 19.90
	ATOM	1427 C LEU 346	61.317 17.806 14.716 1.00 20.19
	ATOM	1428 O LEU 346	62.407 17.755 14.142 1.00 20.69
	ATOM	1429 N LEU 347	60.290 17.016 14.390 1.00 22.00
	ATOM	1430 CA LEU 347	60.406 15.994 13.344 1.00 21.81
25	ATOM	1431 CB LEU 347	59.199 15.051 13.366 1.00 24.03
	ATOM	1432 CG LEU 347	59.301 13.805 14.250 1.00 26.28
	ATOM	1433 CD1 LEU 347	57.964 13.072 14.277 1.00 27.79
	ATOM	1434 CD2 LEU 347	60.409 12.889 13.728 1.00 24.78
	ATOM	1435 C LEU 347	60.544 16.623 11.966 1.00 20.50
30	ATOM	1436 O LEU 347	61.351 16.179 11.143 1.00 21.39
	ATOM	1437 N ALA 348	59.767 17.674 11.727 1.00 20.84
	ATOM	1438 CA ALA 348	59.788 18.381 10.456 1.00 18.12
	ATOM	1439 CB ALA 348	58.729 19.480 10.457 1.00 18.49
	ATOM	1440 C ALA 348	61.168 18.963 10.269 1.00 17.53
35	ATOM	1441 O ALA 348	61.785 18.781 9.228 1.00 18.78
	ATOM	1442 N PHE 349	61.677 19.569 11.338 1.00 19.55
	ATOM	1443 CA PHE 349	63.001 20.196 11.389 1.00 19.84
	ATOM	1444 CB PHE 349	63.188 20.823 12.786 1.00 18.68
	ATOM	1445 CG PHE 349	64.380 21.758 12.917 1.00 19.12
40	ATOM	1446 CD1 PHE 349	65.234 22.008 11.851 1.00 19.95
	ATOM	1447 CD2 PHE 349	64.618 22.420 14.126 1.00 20.06
	ATOM	1448 CE1 PHE 349	66.294 22.905 11.971 1.00 18.99
	ATOM	1449 CE2 PHE 349	65.674 23.317 14.261 1.00 16.79
	ATOM	1450 CZ PHE 349	66.516 23.562 13.184 1.00 18.91
45	ATOM	1451 C PHE 349	64.108 19.170 11.103 1.00 20.44
	ATOM	1452 O PHE 349	64.980 19.401 10.260 1.00 19.83
	ATOM	1453 N GLU 350	64.064 18.032 11.794 1.00 23.59
	ATOM	1454 CA GLU 350	65.077 16.995 11.610 1.00 23.46
* ^	ATOM	1455 CB GLU 350	64.830 15.845 12.584 1.00 25.26
50	ATOM	1456 CG GLU 350	65.694 14.644 12.288 1.00 31.98

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ATOM 1457 CD GLU 350
                                65.526 13.482 13.257 1.00 35.49
     ATOM 1458 OE1 GLU 350
                                 66.560 12.853 13.555 1.00 40.26
     ATOM 1459 OE2 GLU 350
                                 64.380 13.173 13.689 1.00 36.23
     ATOM 1460 C GLU 350
                               65.083 16.489 10.165 1.00 21.12
     ATOM 1461 O GLU 350
                               66.133 16.384 9.526 1.00 19.81
                               63.888 16.234 9.651 1.00 21.98
     ATOM 1462 N HIS 351
                               63.694 15.751 8.292 1.00 21.31
     ATOM 1463 CA HIS 351
     ATOM 1464 CB HIS 351
                               62.238 15.321 8.107 1.00 21.76
     ATOM 1465 CG HIS 351
                               61.839 14.160 8.967 1.00 22.08
     ATOM 1466 CD2 HIS 351
                                62.578 13.317 9.728 1.00 22.65
10
     ATOM 1467 ND1 HIS 351
                                60.532 13.751 9.115 1.00 22.37
     ATOM 1468 CE1 HIS 351
                               60.478 12.716 9.930 1.00 21.44
                                61.705 12.429 10.314 1.00 20.85
     ATOM 1469 NE2 HIS 351
     ATOM 1470 C HIS 351
                              64.117 16.815 7.275 1.00 21.18
15
     ATOM 1471 O HIS 351
                               64.683 16.489 6.231 1.00 22.65
     ATOM 1472 N TYR 352
                               63.915 18.088 7.602 1.00 19.79
     ATOM 1473 CA TYR 352
                                64.327 19.146 6.697 1.00 18.72
     ATOM 1474 CB TYR 352
                                63.768 20.502 7.122 1.00 19.55
                                64.140 21.580 6.137 1.00 19.27
     ATOM 1475 CG TYR 352
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     ATOM 1476 CD1 TYR 352
                                 63.556 21.623 4.867 1.00 19.29
     ATOM 1477 CE1 TYR 352
                                63.961 22.555 3.927 1.00 17.55
     ATOM 1478 CD2 TYR 352
                                65.132 22.507 6.438 1.00 18.91
     ATOM 1479 CE2 TYR 352
                                65.545 23.443 5.503 1.00 17.30
     ATOM 1480 CZ TYR 352
                                64.954 23.459 4.256 1.00 18.41
     ATOM 1481 OH TYR 352
                                65.355 24.384 3.334 1.00 19.40
25
     ATOM 1482 C TYR 352
                               65.849 19.182 6.687 1.00 19.31
     ATOM 1483 O TYR 352
                               66.479 19.333 5.639 1.00 20.25
     ATOM 1484 N VAL 353
                               66.446 19.017 7.858 1.00 21.25
                                67.899 18.993 7.960 1.00 22.03
     ATOM 1485 CA VAL 353
    ATOM 1486 CB VAL 353
                                68.348 18.880 9.450 1.00 22.60
30
     ATOM 1487 CG1 VAL 353
                                 69.843 18.635 9.550 1.00 20.34
    ATOM 1488 CG2 VAL 353
                                 67.997 20.167 10.183 1.00 22.61
    ATOM 1489 C VAL 353
                               68.442 17.827 7.108 1.00 22.74
    ATOM 1490 O VAL 353
                               69.448 17.985 6.398 1.00 23.44
35
    ATOM 1491 N ASN 354
                               67.773 16.674 7.165 1.00 22.30
    ATOM 1492 CA ASN 354
                                68.185 15.508 6.373 1.00 23.56
    ATOM 1493 CB ASN 354
                                67.241 14.320 6.603 1.00 22.26
     ATOM 1494 CG ASN 354
                                67.374 13.715 7.981 1.00 23.06
    ATOM 1495 OD1 ASN 354
                                68.406 13.843 8.628 1.00 25.79
40
    ATOM 1496 ND2 ASN 354
                                 66.327 13.044 8.435 1.00 21.07
    ATOM 1497 C ASN 354
                               68.134 15.877 4.888 1.00 25.10
    ATOM 1498 O ASN 354
                               69.024 15.534 4.111 1.00 26.70
    ATOM 1499 N HIS 355
                              67.067 16.568 4.503 1.00 24.50
    ATOM 1500 CA HIS 355
                               66.881 16.986 3.123 1.00 24.46
    ATOM 1501 CB HIS 355
                               65.557 17.750 2.969 1.00 26.07
45
                               65.365 18.337 1.604 1.00 28.28
    ATOM 1502 CG HIS 355
    ATOM 1503 CD2 HIS 355
                               65.918 19.422 1.018 1.00 28.10
    ATOM 1504 ND1 HIS 355
                                64.600 17.724 0.632 1.00 26.32
    ATOM 1505 CE1 HIS 355
                               64.706 18.407 -0.499 1.00 27.71
    ATOM 1506 NE2 HIS 355
                               65.502 19.435 -0.288 1.00 27.79
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ATOM 1507 C HIS 355
                              68.022 17.857 2.624 1.00 24.07
     ATOM 1508 O HIS 355
                              68.460 17.729 1.484 1.00 23.54
     ATOM 1509 N ARG 356
                               68.463 18.774 3.471 1.00 25.31
     ATOM 1510 CA ARG 356
                                69.523 19.714 3.130 1.00 25.69
                                69.561 20.820 4.168 1.00 24.06
     ATOM 1511 CB ARG 356
                                68.337 21.682 4.094 1.00 23.23
     ATOM 1512 CG ARG 356
                                68.670 22.973 3.424 1.00 25.91
     ATOM 1513 CD ARG 356
                                69,447 23,814 4,322 1,00 24,87
     ATOM 1514 NE ARG 356
                                70.325 24.726 3.928 1.00 25.05
     ATOM 1515 CZ ARG 356
                                 70.546 24.920 2.640 1.00 24.97
     ATOM 1516 NH1 ARG 356
10
                                 70.978 25.453 4.831 1.00 25.62
     ATOM 1517 NH2 ARG 356
                               70.900 19.109 2.949 1.00 27.73
     ATOM 1518 C ARG 356
                               71.724 19.645 2.208 1.00 28.38
     ATOM 1519 O ARG 356
     ATOM 1520 N LYS 357
                               71.179 18.048 3.693 1.00 29.45
     ATOM 1521 CA LYS 357
                                72.457 17.355 3.588 1.00 31.35
15
                                72,503 16.566 2.270 1.00 32.80
     ATOM 1522 CB LYS 357
                                71.290 15.650 2.103 1.00 35.78
     ATOM 1523 CG LYS 357
                                71.264 14.927 0.778 1.00 39.43
     ATOM 1524 CD LYS 357
                                70.121 13.918 0.739 1.00 42.93
     ATOM 1525 CE LYS 357
                                70.162 13.074 -0.498 1.00 45.97
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     ATOM 1526 NZ LYS 357
                               73.692 18.247 3.743 1.00 31.34
     ATOM 1527 C LYS 357
                               74.489 18.390 2.818 1.00 32.65
     ATOM 1528 O LYS 357
                              73.837 18.861 4.913 1.00 30.72
     ATOM 1529 N HIS 358
                               74.995 19.706 5.186 1.00 31.49
     ATOM 1530 CA HIS 358
                               74.895 20.322 6.579 1.00 29.13
25
     ATOM 1531 CB HIS 358
     ATOM 1532 CG HIS 358
                               73.882 21.415 6.688 1.00 25.30
     ATOM 1533 CD2 HIS 358
                                74.026 22.760 6.646 1.00 24.90
     ATOM 1534 ND1 HIS 358
                                72.543 21.175 6.892 1.00 24.54
     ATOM 1535 CE1 HIS 358
                               71.901 22.324 6.975 1.00 23.68
30
     ATOM 1536 NE2 HIS 358
                                72.777 23.302 6.830 1.00 25.28
     ATOM 1537 C HIS 358
                              76.235 18.831 5.161 1.00 33.38
                              76.166 17.647 5.495 1.00 35.46
     ATOM 1538 O HIS 358
     ATOM 1539 N ASN 359
                               77.366 19.399 4.768 1.00 35.34
     ATOM 1540 CA ASN 359
                                78.606 18.636 4.746 1.00 38.17
     ATOM 1541 CB ASN 359
                                79.544 19.150 3.646 1.00 37.84
35
     ATOM 1542 C ASN 359
                               79.236 18.825 6.120 1.00 39.85
                               80.317 19.406 6.240 1.00 42.72
     ATOM 1543 O ASN 359
     ATOM 1544 N ILE 360
                              78.510 18.411 7.159 1.00 39.01
                               78.968 18.526 8.549 1.00 36.72
     ATOM 1545 CA ILE 360
                               78.351 19.752 9.264 1.00 37.69
40
     ATOM 1546 CB ILE 360
     ATOM 1547 CG2 ILE 360
                                78.802 19.793 10.722 1.00 37.56
     ATOM 1548 CG1 ILE 360
                                78.735 21.049 8.549 1.00 37.68
                                77.970 22.253 9.041 1.00 38.40
     ATOM 1549 CD1 ILE 360
                              78.524 17.278 9.303 1.00 35.15
     ATOM 1550 C ILE 360
                              77.343 16.931 9.314 1.00 33.75
45
     ATOM 1551 O ILE 360
                               79.475 16.564 9.912 1.00 34.64
     ATOM 1552 N PRO 361
                                80.930 16.785 9.873 1.00 35.59
     ATOM 1553 CD PRO 361
     ATOM 1554 CA PRO 361
                                79.138 15.349 10.660 1.00 33.92
                                80.513 14.768 11.014 1.00 35.27
     ATOM 1555 CB PRO 361
                                81.412 15.972 11.048 1.00 35.97
50
     ATOM 1556 CG PRO 361
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ATOM 1557 C PRO 361
                               78.292 15.618 11.909 1.00 30.95
     ATOM 1558 O PRO 361
                                78.555 16.554 12.653 1.00 31.50
     ATOM 1559 N HIS 362
                               77.269 14.793 12.112 1.00 28.75
     ATOM 1560 CA HIS 362
                                76.378 14.900 13.263 1.00 30.25
     ATOM 1561 CB HIS 362
                                77.152 14.612 14.548 1.00 31.20
     ATOM 1562 CG HIS 362
                                78.075 13.441 14.440 1.00 33.72
     ATOM 1563 CD2 HIS 362
                                77.826 12.122 14.275 1.00 34.55
     ATOM 1564 ND1 HIS 362
                                79.449 13.569 14.469 1.00 35.55
     ATOM 1565 CE1 HIS 362
                                80.006 12.377 14.322 1.00 35.28
     ATOM 1566 NE2 HIS 362
10
                                79.040 11.484 14.204 1.00 37.61
     ATOM 1567 C HIS 362
                               75.742 16.275 13.368 1.00 29.44
                               75.521 16.769 14.472 1.00 29.93
     ATOM 1568 O HIS 362
     ATOM 1569 N PHE 363
                               75.397 16.856 12.222 1.00 29.22
     ATOM 1570 CA PHE 363
                                74.803 18.188 12.160 1.00 27.72
     ATOM 1571 CB PHE 363
                                74.446 18.538 10.709 1.00 26.85
15
     ATOM 1572 CG PHE 363
                                73.901 19.931 10.532 1.00 27.48
     ATOM 1573 CD1 PHE 363
                                 74.758 21.017 10.391 1.00 27.76
     ATOM 1574 CD2 PHE 363
                                 72.523 20.157 10.513 1.00 27.45
     ATOM 1575 CE1 PHE 363
                                74.244 22.313 10.234 1.00 28.56
20
     ATOM 1576 CE2 PHE 363
                                72.001 21.446 10.357 1.00 25.15
     ATOM 1577 CZ PHE 363
                                72.860 22.521 10.219 1.00 24.41
     ATOM 1578 C PHE 363
                               73.597 18.385 13.075 1.00 27.45
     ATOM 1579 O PHE 363
                               73.577 19.324 13.880 1.00 27.73
     ATOM 1580 N TRP 364
                               72.616 17.489 12.983 1.00 25.89
25
     ATOM 1581 CA TRP 364
                                71.401 17.592 13.800 1.00 25.85
     ATOM 1582 CB TRP 364
                                70.444 16.426 13.506 1.00 24.27
     ATOM 1583 CG TRP 364
                                69.168 16.391 14.328 1.00 23.75
     ATOM 1584 CD2 TRP 364
                                68.152 17.407 14.397 1.00 24.87
     ATOM 1585 CE2 TRP 364
                                67.140 16.922 15.261 1.00 24.81
     ATOM 1586 CE3 TRP 364
                                67.989 18.674 13.820 1.00 25.47
30
     ATOM 1587 CD1 TRP 364
                                68.745 15.370 15.122 1.00 22.98
     ATOM 1588 NE1 TRP 364
                                67.530 15.679 15.684 1.00 25.99
     ATOM 1589 CZ2 TRP 364
                                65.987 17.661 15.560 1.00 25.14
     ATOM 1590 CZ3 TRP 364
                                66.844 19.405 14.116 1.00 25.29
35
     ATOM 1591 CH2 TRP 364
                                65.857 18.894 14.982 1.00 24.53
     ATOM 1592 C TRP 364
                               71.659 17.747 15.308 1.00 26.94
     ATOM 1593 O TRP 364
                               71.202 18.721 15.904 1.00 27.16
     ATOM 1594 N PRO 365
                               72.382 16.796 15.944 1.00 27.60
                                72.912 15.522 15.411 1.00 27.55
     ATOM 1595 CD PRO 365
40
     ATOM 1596 CA PRO 365
                                72.655 16.915 17.387 1.00 25.90
     ATOM 1597 CB PRO 365
                                73.565 15.717 17.668 1.00 26.00
     ATOM 1598 CG PRO 365
                                73.136 14.705 16.658 1.00 28.32
     ATOM 1599 C PRO 365
                               73.374 18.225 17.714 1.00 23.89
     ATOM 1600 O PRO 365
                               73.088 18.861 18.725 1.00 23.81
    ATOM 1601 N LYS 366
                               74,297 18,626 16,845 1,00 24,24
    ATOM 1602 CA LYS 366
                                75.058 19.862 17.027 1.00 26.24
    ATOM 1603 CB LYS 366
                                76.144 19.982 15.963 1.00 27.44
     ATOM 1604 CG LYS 366
                                77.310 19.022 16.138 1.00 28.76
     ATOM 1605 CD LYS 366
                                78.254 19.171 14.975 1.00 30.53
50
    ATOM 1606 CE LYS 366
                                79.527 18.387 15.167 1.00 34.25
```

	ATOM	1607 NZ LYS 366	80.388 18.463 13.947 1.00 37.89
	ATOM	1608 C LYS 366	74.181 21.107 16.993 1.00 26.73
	ATOM	1609 O LYS 366	74.385 22.042 17.762 1.00 27.36
	ATOM	1610 N LEU 367	73.216 21.124 16.086 1.00 27.98
5	ATOM	1611 CA LEU 367	72.308 22.256 15.967 1.00 27.87
_	ATOM	1612 CB LEU 367	71.559 22.192 14.632 1.00 27.29
	ATOM	1613 CG LEU 367	70.613 23.356 14.318 1.00 27.25
	ATOM	1614 CD1 LEU 367	71.334 24.707 14.510 1.00 22.90
	ATOM	1615 CD2 LEU 367	70,081 23.189 12.896 1.00 24.54
10	ATOM	1616 C LEU 367	71.327 22.223 17.134 1.00 29.38
••	ATOM	1617 O LEU 367	70.993 23.249 17.716 1.00 31.09
	ATOM	1618 N LEU 368	70.889 21.026 17.491 1.00 30.38
	ATOM	1619 CA LEU 368	69.962 20.843 18.594 1.00 31.14
	ATOM	1620 CB LEU 368	69.659 19.353 18.731 1.00 32.20
15	ATOM	1621 CG LEU 368	68.247 18.852 19.014 1.00 33.52
13	ATOM	1622 CD1 LEU 368	67.184 19.651 18.267 1.00 31.14
	ATOM	1623 CD2 LEU 368	68.210 17.379 18.632 1.00 33.99
	ATOM	1624 C LEU 368	70.601 21.395 19.876 1.00 32.36
	ATOM	1625 O LEU 368	69.917 21.963 20.730 1.00 32.58
20	ATOM	1626 N MET 369	71.922 21.272 19.985 1.00 33.30
20	ATOM	1627 CA MET 369	72.641 21.771 21.149 1.00 34.04
	ATOM	1628 CB MET 369	74.051 21.190 21.209 1.00 35.31
	ATOM	1629 CG MET 369	74.108 19.858 21.935 1.00 36.83
	ATOM	1630 SD MET 369	75.312 18.728 21.235 1.00 43.07
25	ATOM	1631 CE MET 369	76.862 19.636 21.472 1.00 41.31
23	ATOM	1632 C MET 369	72.675 23.297 21.212 1.00 34.30
	ATOM	1633 O MET 369	72.961 23.876 22.269 1.00 35.82
	ATOM	1634 N LYS 370	72.368 23.949 20.091 1.00 32.14
	ATOM	1635 CA LYS 370	72.325 25.405 20.044 1.00 29.17
30	ATOM	1636 CB LYS 370	72.394 25.904 18.608 1.00 28.18
50	ATOM	1637 CG LYS 370	73.662 25.518 17.900 1.00 27.72
	ATOM	1638 CD LYS 370	74.866 25.969 18.679 1.00 28.10
	ATOM	1639 CE LYS 370	76.127 25.650 17.930 1.00 27.79
	ATOM	1640 NZ LYS 370	77.298 25.941 18.777 1.00 30.78
35	ATOM	1641 C LYS 370	71.033 25.875 20.705 1.00 29.27
	ATOM	1642 O LYS 370	70.950 26.999 21.200 1.00 29.43
	ATOM	1643 N VAL 371	70.018 25.014 20.714 1.00 29.40
	ATOM	1644 CA VAL 371	68.756 25.358 21.358 1.00 29.90
	ATOM	1645 CB VAL 371	67.687 24.237 21.218 1.00 28.75
40	ATOM	1646 CG1 VAL 371	66,463 24.561 22.064 1.00 27.12
	ATOM	1647 CG2 VAL 371	67.275 24.080 19.762 1.00 29.23
	ATOM	1648 C VAL 371	69.075 25.573 22.832 1.00 31.39
	ATOM	1649 O VAL 371	68.543 26.481 23.462 1.00 31.20
	ATOM	1650 N THR 372	69.971 24.743 23.366 1.00 31.39
45	ATOM	1651 CA THR 372	70.371 24.847 24.762 1.00 31.10
	ATOM	1652 CB THR 372	71.282 23.664 25.170 1.00 31.59
	ATOM	1653 OG1 THR 372	70.554 22.441 25.008 1.00 30.60
	ATOM	1654 CG2 THR 372	71.720 23.795 26.625 1.00 30.14
	ATOM	1655 C THR 372	71.071 26.186 24.994 1.00 30.76
50	ATOM	1656 O THR 372	70.711 26.935 25.910 1.00 31.45

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	ATOM	1657 N ASP 373 7	2.038 26.507 24.138 1.00 29.31
	ATOM	1658 CA ASP 373	72.744 27.772 24.252 1.00 27.32
	ATOM		73.745 27.934 23.115 1.00 27.98
	ATOM		74.886 26.933 23.190 1.00 28.94
5	ATOM	1661 OD1 ASP 373	75.043 26.259 24.225 1.00 31.01
	ATOM	1662 OD2 ASP 373	75.639 26.825 22.205 1.00 31.38
	ATOM		1.742 28.926 24.247 1.00 26.50
	ATOM		1.872 29.861 25.040 1.00 27.35
	ATOM		0.711 28.826 23.412 1.00 24.17
10	ATOM		69.688 29.864 23.331 1.00 23.38
	ATOM		68.795 29.660 22.107 1.00 22.98
	ATOM		69.361 30.183 20.786 1.00 24.45
	ATOM	1669 CD1 LEU 374	68.668 29.520 19.589 1.00 24.72
	ATOM	1670 CD2 LEU 374	69.223 31.704 20.735 1.00 22.40
15	ATOM		8.839 29.964 24.589 1.00 24.31
	ATOM		8.442 31.065 24.986 1.00 23.31
	ATOM		58.543 28.826 25.211 1.00 25.32
	ATOM	1674 CA ARG 375	67.748 28.821 26.438 1.00 27.76
	ATOM		67.455 27.392 26.908 1.00 30.82
20	ATOM	1676 CG ARG 375	66.901 26.439 25.854 1.00 38.79
	ATOM	1677 CD ARG 375	65,424 26.630 25,582 1.00 45.40
	ATOM		64.709 25.360 25.620 1.00 52.61
	ATOM		63.800 24.967 24.726 1.00 56.89
	ATOM	1680 NH1 ARG 375	63.473 25.732 23.694 1.00 58.27
25	ATOM	1681 NH2 ARG 375	63.201 23.793 24.855 1.00 58.46
	ATOM		58.563 29.542 27.512 1.00 26.98
	ATOM		58.025 30.336 28.282 1.00 26.18
	ATOM	1684 N MET 376	59.862 29.255 27.551 1.00 26.80
	ATOM	1685 CA MET 376	70.767 29.867 28.511 1.00 29.22
30	ATOM	1686 CB MET 376	72.172 29.270 28.379 1.00 33.70
	ATOM	1687 CG MET 376	72.595 28.371 29.562 1.00 43.20
	ATOM	1688 SD MET 376	73.320 29.260 31.011 1.00 52.38
	ATOM	1689 CE MET 376	71.843 29.854 31.913 1.00 48.11
	ATOM		70.804 31.384 28.339 1.00 27.54
35	ATOM	1691 O MET 376	70.792 32.126 29.323 1.00 26.96
	ATOM	1692 N ILE 377 70	0.841 31.835 27.087 1.00 25.39
	ATOM		0.847 33.264 26.767 1.00 23.26
	ATOM		0.992 33.488 25.222 1.00 22.73
	ATOM		70.560 34.909 24.819 1.00 21.81
40	ATOM	1696 CG1 ILE 377	72.431 33.205 24.789 1.00 20.39
	ATOM		72.644 33.148 23.300 1.00 18.85
	ATOM		2.558 33.900 27.309 1.00 22.91
	ATOM		0.597 34.925 27.989 1.00 22.02
	ATOM		58.427 33.244 27.069 1.00 22.29
45	ATOM	1701 CA GLY 378	67.161 33.757 27.547 1.00 22.83
	ATOM		7.111 33.815 29.063 1.00 25.60
	ATOM		66.546 34.752 29.630 1.00 26.25
	ATOM		57.691 32.804 29.713 1.00 26.88
	ATOM		67.744 32.707 31.175 1.00 27.19
50	ATOM	1706 CB ALA 379	68.322 31.358 31.590 1.00 26.97

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	ATOM	1707 C ALA 379 68.606 33.827 31.738 1.00 26.13
	ATOM	1708 O ALA 379 68.174 34.580 32.601 1.00 26.46
	ATOM	1709 N CYA 380 69.826 33.935 31.230 1.00 27.61
	ATOM	1710 CA CYA 380 70.742 34.973 31.667 1.00 29.74
5	ATOM	1711 CB CYA 380 72.070 34.865 30.923 1.00 35.44
	ATOM	1712 SG CYA 380 73.081 33.458 31.417 1.00 42.61
	ATOM	1713 AS CYA 380 74.829 33.691 29.945 1.00 55.91
	ATOM	1714 C CYA 380 70.142 36.349 31.446 1.00 29.07
	ATOM	1715 O CYA 380 70.243 37.225 32.303 1.00 29.46
10	ATOM	1716 N HIS 381 69.494 36.538 30.304 1.00 28.29
	ATOM	1717 CA HIS 381 68.885 37.824 30.002 1.00 26.84
	ATOM	1718 CB HIS 381 68.384 37.880 28.557 1.00 23.13
	ATOM	1719 CG HIS 381 67.597 39.113 28.259 1.00 19.84
	ATOM	1720 CD2 HIS 381 67.993 40.365 27.931 1.00 18.68
15	ATOM	1721 ND1 HIS 381 66.229 39.169 28.403 1.00 19.47
	ATOM	1722 CE1 HIS 381 65.817 40.407 28.190 1.00 18.64
	ATOM	1723 NE2 HIS 381 66.868 41.149 27.900 1.00 18.29
	ATOM	1724 C HIS 381 67.747 38.157 30.967 1.00 26.78
	ATOM	1725 O HIS 381 67.560 39.314 31.337 1.00 26.39
20	ATOM	1726 N ALA 382 66.964 37.158 31.347 1.00 27.78
	ATOM	1727 CA ALA 382 65.867 37.395 32.269 1.00 29.45
	ATOM	1728 CB ALA 382 65.077 36.125 32.471 1.00 29.51
	ATOM	1729 C ALA 382 66.425 37.904 33.604 1.00 31.74
	ATOM	1730 O ALA 382 65.932 38.882 34.159 1.00 32.60
25	ATOM	1731 N SER 383 67.483 37.262 34.093 1.00 33.02
	ATOM	1732 CA SER 383 68.109 37.662 35.350 1.00 34.69
	ATOM	1733 CB SER 383 69.212 36.677 35.733 1.00 36.18
	ATOM	1734 OG SER 383 68.663 35.386 35.933 1.00 40.61
	ATOM	1735 C SER 383 68.689 39.064 35.242 1.00 33.49
30	ATOM	1736 O SER 383 68.526 39.889 36.146 1.00 34.28
	ATOM	1737 N ARG 384 69.377 39.332 34.141 1.00 32.60
	ATOM	1738 CA ARG 384 69.955 40.642 33.938 1.00 32.60
	ATOM	1739 CB ARG 384 70.926 40.638 32.762 1.00 33.60
	ATOM	1740 CG ARG 384 71.429 42.013 32.409 1.00 36.33
35	ATOM	1741 CD ARG 384 72.875 41.975 31.993 1.00 39.62
	ATOM	1742 NE ARG 384 73.760 42.260 33.114 1.00 41.76
	ATOM	1743 CZ ARG 384 74.587 43.301 33.179 1.00 41.92
	ATOM	1744 NH1 ARG 384 74.670 44.182 32.191 1.00 40.66
	ATOM	1745 NH2 ARG 384 75.319 43.471 34.260 1.00 44.88
40	ATOM	1746 C ARG 384 68.862 41.694 33.758 1.00 32.28
	ATOM	1747 O ARG 384 69.014 42.831 34.213 1.00 33.27
	ATOM	1748 N PHE 385 67.739 41.311 33.159 1.00 29.13
	ATOM	1749 CA PHE 385 66.663 42.259 32.977 1.00 27.55
	ATOM	1750 CB PHE 385 65.552 41.687 32.105 1.00 26.89
45	ATOM	1751 CG PHE 385 64.415 42.641 31.888 1.00 25.11
	ATOM	1752 CD1 PHE 385 64.495 43.630 30.918 1.00 24.94
	ATOM	1753 CD2 PHE 385 63.281 42.580 32.689 1.00 25.01
	ATOM	1754 CE1 PHE 385 63.466 44.547 30.753 1.00 25.50
	ATOM	1755 CE2 PHE 385 62.244 43.495 32.531 1.00 24.06
50	ATOM	1756 CZ PHE 385 62.338 44.482 31.563 1.00 25.44

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66.125 42.641 34.348 1.00 29.08
    ATOM 1757 C PHE 385
                               65.887 43.816 34.613 1.00 27.90
    ATOM 1758 O PHE 385
                               65.972 41.658 35.231 1.00 31.19
    ATOM 1759 N LEU 386
                                65.465 41.929 36.577 1.00 33.22
    ATOM 1760 CA LEU 386
                                65,355 40,640 37.397 1.00 34.35
    ATOM 1761 CB LEU 386
                               66.362 42.940 37.279 1.00 33.52
    ATOM 1762 C LEU 386
    ATOM 1763 O LEU 386
                               65.874 43.907 37.855 1.00 32.93
                              67.673 42.760 37.158 1.00 34.80
    ATOM 1764 N HIS 387
                               68.628 43.674 37.775 1.00 37.88
    ATOM 1765 CA HIS 387
                               70.042 43.112 37.705 1.00 36.66
    ATOM 1766 CB HIS 387
10
                               70.206 41.832 38.456 1.00 39.14
    ATOM 1767 CG HIS 387
    ATOM 1768 CD2 HIS 387
                                69.307 41.080 39.144 1.00 39.28
    ATOM 1769 ND1 HIS 387
                                71.408 41.161 38.543 1.00 40.97
    ATOM 1770 CE1 HIS 387
                                71.241 40.055 39.245 1.00 41.57
    ATOM 1771 NE2 HIS 387
                                69.980 39.984 39.618 1.00 41.45
15
                              68.589 45.071 37.164 1.00 40.38
    ATOM 1772 C HIS 387
                              68.673 46.054 37.888 1.00 40.87
    ATOM 1773 O HIS 387
                               68.466 45.161 35.842 1.00 43.32
    ATOM 1774 N MET 388
                                68.398 46.455 35.168 1.00 46.28
    ATOM 1775 CA MET 388
                                68.170 46.286 33.665 1.00 43.30
20
    ATOM 1776 CB MET 388
    ATOM 1777 CG MET 388
                                69.342 45.738 32.875 1.00 43.55
    ATOM 1778 SD MET 388
ATOM 1779 CE MET 388
                                69.034 45.896 31.098 1.00 46.27
                                68.208 44.370 30.709 1.00 42.36
    ATOM 1780 C MET 388
                               67.256 47.289 35.737 1.00 50.25
                                67.363 48.506 35.886 1.00 49.79
    ATOM 1781 O MET 388
25
                               66.163 46.610 36.075 1.00 52.74
     ATOM 1782 N LYS 389
                                                              ALTA
    ATOM 1783 CA LYS 389
                                64.983 47.274 36.633 1.00 56.15
                                                               ALTA
     ATOM 1784 CB LYS 389
                                63.770 46.334 36.565 1.00 56.87
                                                               ALTA
     ATOM 1785 CG LYS 389
                                63.227 46.087 35.161 1.00 57.76
                                                               ALTA
                                62.029 45.156 35.212 1.00 55.98
    ATOM 1786 CD LYS 389
                                                               ALTA
30
     ATOM 1787 CE LYS 389
                                62.426 43.796 35.778 1.00 55.48
                                                               ALTA
     ATOM 1788 NZ LYS 389
                                61.267 43.040 36.311 1.00 55.55
                                                               ALTA
                               65,177 47,767 38.064 1.00 56.69
                                                              ALTA
     ATOM 1789 C LYS 389
                               64.623 48.814 38.453 1.00 58.54
                                                              ALTA
     ATOM 1790 O LYS 389
                               65.955 47.038 38.839 1.00 55.21
     ATOM 1791 N VAL 390
35
     ATOM 1792 CA VAL 390
                                66.225 47.386 40.236 1.00 51.78
                                66.999 46.231 40.985 1.00 50.07
     ATOM 1793 CB VAL 390
                                 67.648 46.726 42.263 1.00 49.74
     ATOM 1794 CG1 VAL 390
     ATOM 1795 CG2 VAL 390
                                 66.037 45.093 41.317 1.00 49.06
                               67.053 48.681 40.227 1.00 49.38
40
     ATOM 1796 C VAL 390
                                66.785 49.605 40.992 1.00 48.71
     ATOM 1797 O VAL 390
                                67.974 48.778 39.272 1.00 46.71
     ATOM 1798 N GLU 391
                                68.866 49.919 39.142 1.00 44.88
     ATOM 1799 CA GLU 391
     ATOM 1800 CB GLU 391
                                70.156 49.488 38.438 1.00 45.24
                                70.793 48.207 38.997 1.00 47.65
45
     ATOM 1801 CG GLU 391
     ATOM 1802 CD GLU 391
                                71.461 48.388 40.358 1.00 50.29
     ATOM 1803 OE1 GLU 391
                                71.141 49.373 41.063 1.00 50.68
     ATOM 1804 OE2 GLU 391
                                72.310 47.535 40.718 1.00 50.85
                               68.324 51.174 38.458 1.00 45.28
     ATOM 1805 C GLU 391
                                68.568 52.286 38.940 1.00 46.46
50
     ATOM 1806 O GLU 391
```

	ATOM	1807 N CYA 392	67.568 51.024 37.372 1.00 43.33
	ATOM	1808 CA CYA 392	67.071 52.192 36.643 1.00 42.28
	ATOM	1809 CB CYA 392	67.519 52.096 35.197 1.00 42.45
	ATOM	1810 SG CYA 392	69.280 52.182 35.127 1.00 43.69
5	ATOM	1811 AS CYA 392	69.908 51.044 33.336 1.00 48.17
	ATOM	1812 C CYA 392	65.589 52.493 36.709 1.00 42.51
	ATOM	1813 O CYA 392	64.792 51.634 37.070 1.00 43.30
	ATOM	1814 N PRO 393	65.205 53.752 36.418 1.00 42.13
	ATOM	1815 CD PRO 393	66.109 54.899 36.199 1.00 40.54
10	ATOM	1816 CA PRO 393	63.794 54.182 36.441 1.00 42.26
	ATOM	1817 CB PRO 393	63.896 55.710 36.365 1.00 41.47
	ATOM	1818 CG PRO 393	65.189 55.938 35.614 1.00 41.10
	ATOM	1819 C PRO 393	62.954 53.606 35.281 1.00 43.20
	ATOM	1820 O PRO 393	63.463 53.452 34.163 1.00 42.61
15	ATOM	1821 N THR 394	61.686 53.305 35.559 1.00 43.70
	ATOM	1822 CA THR 394	60.764 52.755 34.564 1.00 45.50
	ATOM	1823 CB THR 394	59.340 52.609 35.129 1.00 47.20
	ATOM	1824 OG1 THR 394	59.304 53.139 36.464 1.00 50.57
	ATOM	1825 CG2 THR 394	58.878 51.150 35.137 1.00 47.99
20	ATOM	1826 C THR 394	60.682 53.583 33.283 1.00 44.58
	ATOM	1827 O THR 394	60.409 53.054 32.215 1.00 46.36
	ATOM	1828 N GLU 395	60.899 54.888 33.396 1.00 42.88
	ATOM	1829 CA GLU 395	60.842 55.790 32.246 1.00 40.54
	ATOM	1830 CB GLU 395	61.096 57.234 32.699 1.00 40.69
25	ATOM	1831 C GLU 395	61,799 55.421 31.098 1.00 38.51
	ATOM	1832 O GLU 395	61.628 55.877 29.968 1.00 39.41
	ATOM	1833 N LEU 396	62.828 54.640 31.402 1.00 35.60
	ATOM	1834 CA LEU 396	63.795 54.220 30.386 1.00 33.11
	ATOM	1835 CB LEU 396	65.169 54.003 31.027 1.00 33.60
30	ATOM	1836 CG LEU 396	65,831 55.230 31.660 1.00 34.54
50	ATOM	1837 CD1 LEU 396	67.160 54.835 32.282 1.00 32.83
	ATOM	1838 CD2 LEU 396	66.026 56.308 30.599 1.00 35.71
	ATOM	1839 C LEU 396	63.388 52.940 29.660 1.00 30.95
	ATOM	1840 O LEU 396	63.950 52.605 28.624 1.00 30.90
35	ATOM	1841 N PHE 397	62.422 52.227 30.223 1.00 30.18
55	ATOM	1842 CA PHE 397	61.961 50.970 29.654 1.00 28.80
	ATOM	1843 CB PHE 397	61.712 49.946 30.777 1.00 28.10
	ATOM	1844 CG PHE 397	62.938 49.604 31.592 1.00 28.96
	ATOM	1845 CD1 PHE 397	63.403 50.472 32.591 1.00 28.39
40	ATOM	1846 CD2 PHE 397	63.636 48.422 31.359 1.00 26.28
-10	ATOM	1847 CE1 PHE 397	64.546 50.166 33.337 1.00 28.44
	ATOM	1848 CE2 PHE 397	64.784 48.107 32.103 1.00 29.21
	ATOM	1849 CZ PHE 397	65.240 48.984 33.096 1.00 27.37
	ATOM	1850 C PHE 397	60.683 51.093 28.836 1.00 27.54
45	ATOM	1851 O PHE 397	59.630 51.431 29.370 1.00 26.96
73	ATOM	1852 N PRO 398	60.753 50.836 27.501 1.00 27.41
	ATOM	1853 CD PRO 398	61.968 50.600 26.686 1.00 25.42
	ATOM	1854 CA PRO 398	59.560 50.920 26.654 1.00 25.90
	ATOM	1855 CB PRO 398	60.068 50.383 25.320 1.00 25.26
50	ATOM	1856 CG PRO 398	61.490 50.893 25.290 1.00 23.99
20	ATOM	1030 CG FRO 390	01,770 20.073 23.270 1.00 23.77

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58.494 49.995 27.272 1.00 25.86
    ATOM 1857 C PRO 398
                               58.839 48.962 27.843 1.00 25.82
    ATOM 1858 O PRO 398
                               57.197 50.355 27.175 1.00 25.52
    ATOM 1859 N PRO 399
                                56.627 51.576 26.578 1.00 25.49
    ATOM 1860 CD PRO 399
                                56.145 49.510 27.754 1.00 25.42
    ATOM 1861 CA PRO 399
                                54.861 50.181 27.273 1.00 26.23
     ATOM 1862 CB PRO 399
                                55.237 51.609 27.156 1.00 25.25
    ATOM 1863 CG PRO 399
                               56.198 48.043 27.317 1.00 26.08
    ATOM 1864 C PRO 399
                               56.132 47.131 28.159 1.00 25.45
    ATOM 1865 O PRO 399
                               56.350 47.810 26.019 1.00 25.57
10
    ATOM 1866 N LEU 400
                                56.406 46.440 25.509 1.00 26.27
    ATOM 1867 CA LEU 400
    ATOM 1868 CB LEU 400
                                56.404 46.418 23.980 1.00 25.03
                                56.117 45.042 23.363 1.00 24.51
    ATOM 1869 CG LEU 400
    ATOM 1870 CD1 LEU 400
                                54.757 44.530 23.806 1.00 23.22
     ATOM 1871 CD2 LEU 400
                                 56,173 45,149 21,862 1,00 23,70
15
                               57.602 45.657 26.067 1.00 27.06
     ATOM 1872 C LEU 400
                               57.484 44.465 26.363 1.00 27.41
    ATOM 1873 O LEU 400
                               58.736 46.339 26.231 1.00 27.16
     ATOM 1874 N PHE 401
     ATOM 1875 CA PHE 401
                                59.966 45.754 26.779 1.00 27.06
     ATOM 1876 CB PHE 401
                                61.047 46.833 26.802 1.00 26.60
20
     ATOM 1877 CG PHE 401
                                62.408 46.351 27.217 1.00 28.08
                                62.918 45.138 26.747 1.00 27.45
     ATOM 1878 CD1 PHE 401
     ATOM 1879 CD2 PHE 401
                                63.223 47.165 28.013 1.00 27.48
                                64.220 44.746 27.055 1.00 26.95
     ATOM 1880 CE1 PHE 401
     ATOM 1881 CE2 PHE 401
                                64.523 46.786 28.327 1.00 27.97
25
     ATOM 1882 CZ PHE 401
                                65.028 45.575 27.846 1.00 28.46
                               59.690 45.247 28.205 1.00 27.62
     ATOM 1883 C PHE 401
                               60.046 44.125 28.570 1.00 26.24
     ATOM 1884 O PHE 401
     ATOM 1885 N LEU 402
                               59.036 46.082 29.002 1.00 28.75
     ATOM 1886 CA LEU 402
                                58.692 45.719 30.366 1.00 29.58
30
     ATOM 1887 CB LEU 402
                                58.064 46.910 31.088 1.00 30.04
     ATOM 1888 CG LEU 402
                                59.025 47.974 31.594 1.00 30.14
     ATOM 1889 CD1 LEU 402
                                 58.270 49.263 31.880 1.00 29.61
                                59.734 47.438 32.827 1.00 27.99
     ATOM 1890 CD2 LEU 402
     ATOM 1891 C LEU 402
                               57.693 44.583 30.368 1.00 30.10
35
                               57.836 43.631 31.121 1.00 29.78
     ATOM 1892 O LEU 402
     ATOM 1893 N GLU 403
                               56.688 44.683 29.510 1.00 30.49
                                55,646 43,671 29,453 1.00 32,60
     ATOM 1894 CA GLU 403
                                54.562 44.094 28.469 1.00 37.01
     ATOM 1895 CB GLU 403
     ATOM 1896 CG GLU 403
                                53.329 43.218 28.520 1.00 44.01
40
     ATOM 1897 CD GLU 403
                                52.263 43.632 27.523 1.00 48.50
                                 52.516 44.525 26.677 1.00 49.66
     ATOM 1898 OE1 GLU 403
     ATOM 1899 OE2 GLU 403
                                 51.157 43.050 27.594 1.00 53.06
                               56.083 42.237 29.151 1.00 32.03
     ATOM 1900 C GLU 403
                                55.627 41.304 29.816 1.00 32.58
     ATOM 1901 O GLU 403
45
                                56.955 42.078 28.159 0.50 31.51
     ATOM 1902 N VAL 404
                                                              ALTA
                                57.450 40.765 27.739 0.50 30.96
                                                               ALTA
     ATOM 1903 CA VAL 404
                                58.108 40.849 26.333 0.50 30.32
                                                               ALTA
     ATOM 1904 CB VAL 404
                                 58.616 39.489 25.889 0.50 28.72
     ATOM 1905 CG1 VAL 404
                                                                ALTA
     ATOM 1906 CG2 VAL 404
                                 57.115 41.388 25.328 0.50 31.67
                                                                ALTA
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```

```
ALTA
    ATOM 1907 C VAL 404
                               58.465 40.149 28.696 0.50 30.45
                               58.549 38.926 28.822 0.50 30.10
                                                              ALTA
     ATOM 1908 O VAL 404
                               59,224 41.002 29.369 1.00 30.16
     ATOM 1909 N PHE 405
                                60.266 40.549 30.263 1.00 30.65
    ATOM 1910 CA PHE 405
    ATOM 1911 CB PHE 405
                                61.577 41.221 29.863 1.00 28.92
                                62.062 40.834 28.493 1.00 26.31
     ATOM 1912 CG PHE 405
                                62.342 41.804 27.543 1.00 25.72
    ATOM 1913 CD1 PHE 405
                                62.269 39.500 28.166 1.00 25.92
     ATOM 1914 CD2 PHE 405
                                62.827 41.456 26.278 1.00 26.78
    ATOM 1915 CE1 PHE 405
                                62.752 39.139 26.910 1.00 25.39
10
    ATOM 1916 CE2 PHE 405
                                63.034 40.122 25.962 1.00 24.39
    ATOM 1917 CZ PHE 405
    ATOM 1918 C PHE 405
                               60.011 40.674 31.771 1.00 32.10
     ATOM 1919 O PHE 405
                               60.903 40.237 32.533 1.00 33.88
                                 58.936 41.169 32.188 1.00 34.95
    ATOM 1920 OXT PHE 405
                               67.542 37.066 11.311 1.00 26.83
     ATOM
             1 O1 HOH 501
15
     ATOM
             3 O1 HOH 502
                               68.713 41.227 12.821 1.00 23.42
    ATOM
             2 O1 HOH 503
                               64.446 40.325 12.123 1.00 22.84
             4 O1 HOH 504
                               62.236 39.752 15.941 1.00 17.97
     ATOM
             5 O1 HOH 505
                               48.732 20.137 5.515 1.00 50.48
    ATOM
             6 O1 HOH 506
                               47.365 21.522 3.716 1.00 53.40
20
    ATOM
             7 O1 HOH 507
                               50.211 23.203 7.900 1.00 32.66
     ATOM
                               51.043 20.258 8.253 1.00 21.81
     ATOM
             8 O1 HOH 508
     ATOM
             9 O1 HOH 509
                               48.225 18.176 7.905 1.00 38.96
                              49.569 20.871 11.586 1.00 32.97
             10 O1 HOH 510
     ATOM
                               53.732 17.159 10.856 1.00 47.20
             11 O1 HOH 511
25
     ATOM
     ATOM
             12 O1 HOH 512
                               56.201 16.223 12.164 1.00 18.50
                               56.653 12.298 10.528 1.00 27.71
     ATOM
             13 O1 HOH 513
             14 O1 HOH 514
                               58.661 10.694 9.014 1.00 46.73
     ATOM
                               62.950 10.692 11.952 1.00 43.05
     ATOM
             15 O1 HOH 515
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30
    ATOM
             16 O1 HOH 516
                               68.949 13.188 12.029 1.00 39.28
    ATOM
             17 O1 HOH 517
                               71.997 15.171 8.362 1.00 49.69
             18 O1 HOH 518
     ATOM
             19 O1 HOH 519
                               71.946 17.928 6.743 1.00 24.50
     ATOM
             20 O1 HOH 520
                               75.117 15.684 9.377 1.00 35.98
     ATOM
                               76.677 12.815 10.294 1.00 49.33
             21 O1 HOH 521
35
     ATOM
                               81.421 15.415 15.139 1.00 46.74
     ATOM
             22 O1 HOH 522
                               78.784 21.696 17.564 1.00 49.01
             23 O1 HOH 523
     ATOM
                               79.954 24.822 17.152 1.00 42.91
     ATOM
             24 O1 HOH 524
                               82.199 30.253 18.821 1.00 40.27
     ATOM
             25 O1 HOH 525
                               82.862 33.444 21.988 1.00 46.81
40
     ATOM
             26 O1 HOH 526
                               76.608 30.793 23.452 1.00 46.22
             27 O1 HOH 527
     ATOM
                               74.726 30.483 25.469 1.00 43.76
     ATOM
             28 O1 HOH 528
     ATOM
             29 O1 HOH 529
                               77.059 28.762 20.900 1.00 33.67
             30 O1 HOH 530
                               75.935 33.279 12.269 1.00 25.26
     ATOM
                               77.402 34.447 10.087 1.00 37.04
45
     ATOM
             31 O1 HOH 531
                               74.054 29.941 9.998 1.00 26.86
     ATOM
             32 O1 HOH 532
                               69.544 32.658 7.572 1.00 40.34
     ATOM
             33 O1 HOH 533
                               66.709 33.618 8.477 1.00 20.63
     ATOM
             34 O1 HOH 534
                               68.073 35.828 8.931 1.00 23.99
     ATOM
             35 O1 HOH 535
                               61.865 45.643 14.011 1.00 40.43
50
     ATOM
             36 O1 HOH 536
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	ATOM	37 O1 HOH	537	63.662 46.881 15.670 1.00 28.04
	ATOM	38 O1 HOH	538	63.391 49.310 13.883 1.00 39.59
	ATOM	39 O1 HOH	539	63.491 50.570 10.631 1.00 52.34
	ATOM	40 O1 HOH	540	64.592 46.849 10.299 1.00 26.63
5	ATOM	41 O1 HOH	541	55.575 41.632 10.980 1.00 38.06
3	ATOM	42 O1 HOH	542	51.631 42.062 17.343 1.00 45.99
	ATOM	43 O1 HOH	543	52.755 43.156 20.209 1.00 34.17
	ATOM	44 O1 HOH	544	57.061 49.627 24.004 1.00 24.09
	ATOM	45 O1 HOH	545	61.040 50.561 21.351 1.00 30.91
10	ATOM	46 O1 HOH	546	68.533 53.616 18.390 1.00 30.91
10	ATOM	47 O1 HOH	547	63.371 58.813 29.014 1.00 59.25
	ATOM	48 O1 HOH	548	57.934 52.905 31.175 1.00 40.12
	ATOM	49 O1 HOH	549	62.364 50.496 37.543 1.00 52.28
	ATOM	50 O1 HOH	550	62.256 49.704 40.891 1.00 54.18
15	ATOM	51 O1 HOH	551	61.994 46.430 40.384 1.00 43.84
15	ATOM	52 O1 HOH	552	63.675 44.459 39.268 1.00 44.73
	ATOM	53 O1 HOH	553	58.405 43.920 33.936 1.00 42.88
	ATOM	54 O1 HOH	554	62.863 39.071 34.046 1.00 45.07
	ATOM	55 O1 HOH	555	64.426 36.925 28.676 1.00 25.36
20	ATOM	56 O1 HOH	556	62.375 35.807 26.610 1.00 21.14
	ATOM	57 O1 HOH	557	63.684 33.760 25.609 1.00 33.03
	ATOM	58 O1 HOH	558	61.542 29.906 24.568 1.00 57.37
	ATOM	59 O1 HOH	559	62.353 27.540 24.855 1.00 39.63
	ATOM	60 O1 HOH	560	62.814 28.785 27.536 1.00 58.40
25	ATOM	61 O1 HOH	561	65.531 30.642 28.821 1.00 54.44
	ATOM	62 O1 HOH	562	63.423 24.645 32.964 1.00 50.75
	ATOM	63 O1 HOH	563	64.697 21.149 28.711 1.00 51.41
	ATOM	64 O1 HOH	564	67.100 23.370 26.900 1.00 52.36
	ATOM	65 O1 HOH	565	65.582 20.422 23.303 1.00 40.32
30	ATOM	66 O1 HOH	566	61.577 18.167 23.386 1.00 65.08
	ATOM	67 O1 HOH	567	61.022 22.649 25.573 1.00 48.85
	ATOM	68 O1 HOH	568	57.919 21.446 25.147 1.00 43.39
	ATOM	69 O1 HOH	569	59.435 20.179 28.543 1.00 51.41
	ATOM	70 O1 HOH	570	53.860 23.216 30.984 1.00 50.28
35	ATOM	71 O1 HOH	571	52.825 24.880 32.696 1.00 43.96
	ATOM	72 O1 HOH	572	48.228 29.683 30.486 1.00 44.51
	ATOM	73 O1 HOH	573	48.925 34.467 30.521 1.00 36.28
	ATOM	74 O1 HOH	574	50.766 40.547 29.178 1.00 51.45
	ATOM	75 O1 HOH	575	57.058 32.490 30.420 1.00 31.03
40	ATOM	76 O1 HOH	576	58.075 29.544 24.664 1.00 19.54
	ATOM	77 O1 HOH	577	47.451 19.292 28.703 1.00 33.04
	ATOM	78 O1 HOH	578	53.120 15.471 17.478 1.00 35.68
	ATOM	79 O1 HOH	579	55.101 14.146 16.095 1.00 50.46
	ATOM	80 O1 HOH	580	53.726 14.016 9.059 1.00 41.44
45	ATOM	81 O1 HOH	581	57.223 13.820 1.435 1.00 48.31
	ATOM	82 O1 HOH	582	61.169 15.688 0.210 1.00 17.60
	ATOM	83 O1 HOH	583	67.411 16.019 -0.314 1.00 23.93
	ATOM	84 O1 HOH	584	67.033 17.221 -2.796 1.00 26.21
	ATOM	85 O1 HOH	585	69.893 19.520 -1.582 1.00 59.67
50	ATOM	86 O1 HOH	586	68.489 22.464 0.350 1.00 37.85

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65.794 23.354 0.823 1.00 27.38
             87 O1 HOH 587
    ATOM
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             88 O1 HOH 588
    ATOM
                                64.646 28.208 3.323 1.00 36.74
             89 O1 HOH 589
    ATOM
                               67.215 31.103 3.174 1.00 30.29
             90 O1 HOH 590
     ATOM
                                64.164 35.667 6.220 1.00 39.72
5
    ATOM
             91 O1 HOH 591
                                62.810 37.518 4.836 1.00 48.48
             92 O1 HOH 592
     ATOM
                                68.105 36.898 6.110 1.00 58.00
             93 O1 HOH 593
     ATOM
                                57.390 37.485 2.631 1.00 37.29
     ATOM
             94 O1 HOH 594
                                53.088 36.068 3.949 1.00 50.10
    ATOM
             95 O1 HOH 595
                                52.974 34.676 6.758 1.00 42.52
     ATOM
             96 O1 HOH 596
10
                                58.581 31.465 2.076 1.00 32.18
     ATOM
             97 O1 HOH 597
                                52.786 23.277 1.357 1.00 28.98
     ATOM
             98 O1 HOH 598
                                47.501 26.551 7.672 1.00 47.83
             99 O1 HOH 599
     ATOM
                                46.411 35.754 14.049 1.00 53.46
             100 O1 HOH 600
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     ATOM
15
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     ATOM
                                62.232 9.378 3.311 1.00 35.65
            103 O1 HOH 603
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                                82.807 43.437 17.940 1.00 39.28
     ATOM
            106 O1 HOH 606
20
            107 O1 HOH 607
                                83.882 45.673 20.638 1.00 41.64
     ATOM
                                80.215 41.021 23.441 1.00 43.16
            108 O1 HOH 608
     ATOM
                                79.459 46.296 31.165 1.00 32.40
            109 O1 HOH 609
     ATOM
                                81.880 47.681 33.923 1.00 46.96
            110 O1 HOH 610
     ATOM
                                75.594 46.142 30.384 1.00 28.64
25
     ATOM
            111 O1 HOH 611
                                77.118 40.568 32.575 1.00 34.21
             112 O1 HOH 612
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             113 O1 HOH 613
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                                75.955 56.565 28.863 1.00 46.31
             114 O1 HOH 614
     ATOM
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             115 O1 HOH 615
     ATOM
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            116 O1 HOH 616
     ATOM
30
                                72.726 25.005 29.671 1.00 62.84
            117 O1 HOH 617
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     ATOM 2038 C ACY 701
                                53.721 39.649 24.298 1.00 47.12
     ATOM 2039 O ACY 701
                                  51.652 40.521 24.172 1.00 46.96
     ATOM 2040 OXT ACY 701
     ATOM 2041 CH3 ACY 701
                                  52.600 40.162 26.329 1.00 45.99
35
                              66.961 42.243 18.491 1.00 22.34
     ATOM 2050 C1 T3
                              68.748 43.593 23.015 1.00 21.84
     ATOM 2051 C2 T3
                              66.873 43.557 18.970 1.00 23.43
     ATOM 2052 C3 T3
                              69.252 44.540 23.871 1.00 22.31
     ATOM 2053 C4 T3
                              67.638 43.989 20.011 1.00 24.83
     ATOM 2054 C5 T3
40
                          1
                              68.851 44.553 25.178 1.00 25.16
     ATOM 2055 C6 T3
                          1
     ATOM 2056 C7 T3
                              68.541 43.108 20.632 1.00 24.65
                          1
                              67.895 43.567 25.639 1.00 21.93
     ATOM 2057 C8 T3
                          1
                              68.665 41.792 20.183 1.00 25.09
     ATOM 2058 C9 T3
                          1
                               67.427 42.654 24.733 1.00 23.66
                           1
45
     ATOM 2059 C10 T3
                               67.878 41.380 19.117 1.00 23.12
     ATOM 2060 C11 T3
                           1
                               67.829 42.624 23.384 1.00 19.67
     ATOM 2061 C12 T3
                           1
                               66.055 41.788 17.371 1.00 18.97
     ATOM 2062 C13 T3
                           1
                               66.721 40.956 16.295 1.00 19.32
     ATOM 2063 C15 T3
                           1
                               65.901 40.829 15.051 1.00 19.02
50
     ATOM 2064 C17 T3
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67.393 45.986 20.621 1.00 25.29
ATOM 2065 I1 T3
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ATOM 2066 I2 T3
                    1
ATOM 2067 I3 T3
                    1
                        70.019 40.450 20.975 1.00 25.67
                         68.131 41.337 16.037 1.00 15.12
ATOM 2068 N1 T3
                    1
                         67.542 43.587 26.966 1.00 21.79
ATOM 2069 O1 T3
                     1
ATOM 2070 O2 T3
                     1
                         69.259 43.600 21.682 1.00 22.05
                         66.504 40.852 13.963 1.00 20.38
ATOM 2071 O3 T3
                     1
ATOM 2072 O4 T3
                         64.675 40.731 15.192 1.00 20.16
END
```

WO 99/26966

PCT/US98/25296

APPENDIX 7

TRBTRIAC.PDB

REMARK TR-beta Triac Full length numbering

REMARK refinement resolution: 100 - 2.9 A r= 0.273258 free_r= 0.333794

5 REMARK wa= 5.78307

REMARK target= mlf cycles= 1 steps= 25

REMARK a= 68.72 b= 68.72 c= 130.092 alpha= 90 beta= 90 gamma= 120

REMARK ncs= none

REMARK initial B-factor correction: "none"

10 REMARK ALA 199 to ALA 201 from His-tag

REMARK

REMARK Four cacodylate-modified cysteines (CYA)

REMARK Cys294, Cys298, Cys388, Cys434

REMARK cacodylate modeled as single arsenic atom

15 REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK amino acid sequence confirmed,

20 REMARK differing from that reported by Weinberger et. al.

REMARK in the following codons:

REMARK 243 Pro - Arg

REMARK 337 lle - Thr

REMARK 451 Leu - Phe

25 REMARK as reported by Sakurai et. al.

REMARK note also correction of initiation codon,

REMARK yielding a polypeptide of 461 amino acids

JRNL AUTH A.SAKURAI, A.NAKAI, L.J. DEGROOT

JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE

30 RECEPTOR

JRNL TITL2 BETA GENE

JRNL REF MOL.CELL.ENDO. V.71 1990

JRNL AUTH

C.WEINBERGER,

C.C.THOMPSON,R.LEBO,D.J.GRUOL,R.M.EVANS

35 JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE RECEPTOR

JRNL REF NATURE

V.324 6098 1986

	ATOM	1 CB ALA 199	31.247 28.289 43.613 1.00 71.30	PROT
	ATOM	2 C ALA 199	32.916 26.485 44.170 1.00 68.99	PROT
40	ATOM	3 O ALA 199	33.485 25.410 43.976 1.00 63.84	PROT
	ATOM	4 N ALA 199	30.462 25.993 44.096 1.00 75.00	PROT
	ATOM	5 CA ALA 199	31.571 26.795 43.497 1.00 73.24	PROT
	ATOM	6 N ALA 200	33.419 27.432 44.958 1.00 73.81	PROT
	ATOM	7 CA ALA 200	34.686 27.251 45.658 1.00 67.87	PROT
45	ATOM	8 CB ALA 200	35.182 28.583 46.203 1.00 62.83	PROT
	ATOM	9 C ALA 200	34.539 26.239 46.791 1.00 63.23	PROT
	ATOM	10 O ALA 200	35.486 25.986 47.534 1.00 59.14	PROT

	ATOM	11 N ALA 201	33.345 25.670 46.932 1.00 56.98	PROT
	ATOM	12 CA ALA 201	33.117 24.664 47.957 1.00 51.46	PROT
	ATOM	13 CB ALA 201	31.776 23.992 47.744 1.00 40.35	PROT
	ATOM	14 C ALA 201	34.248 23.662 47.762 1.00 53.15	PROT
5	ATOM	15 O ALA 201	34.624 22.938 48.679 1.00 54.90	PROT
,	ATOM	16 N GLU 202	34.789 23.645 46.546 1.00 44.13	PROT
	ATOM	17 CA GLU 202	35.891 22.767 46.190 1.00 37.47	PROT
	ATOM	18 CB GLU 202	36.086 22.760 44.671 1.00 37.74	PROT
	ATOM	19 CG GLU 202	37.060 21.702 44.173 1.00 57.14	PROT
10	ATOM	20 CD GLU 202	36.457 20.303 44.140 1.00 61.74	PROT
	ATOM	21 OE1 GLU 202	35.211 20.175 44.133 1.00 63.81	PROT
	ATOM	22 OE2 GLU 202	37.236 19.327 44.115 1.00 65.54	PROT
	ATOM	23 C GLU 202	37.156 23.266 46.878 1.00 35.54	PROT
	ATOM	24 O GLU 202	37.874 22.492 47.510 1.00 32.70	PROT
15	ATOM	25 N GLU 203	37.415 24.566 46.755 1.00 31.79	PROT
	ATOM	26 CA GLU 203	38.588 25.188 47.366 1.00 33.63	PROT
	ATOM	27 CB GLU 203	38.603 26.683 47.079 1.00 28.28	PROT
	ATOM	28 C GLU 203	38.588 24.948 48.869 1.00 33.86	PROT
	ATOM	29 O GLU 203	39.644 24.818 49.485 1.00 33.10	PROT
20	ATOM	30 N LEU 204	37.393 24.898 49.451 1.00 34.15	PROT
	ATOM	31 CA LEU 204	37.244 24.650 50.876 1.00 33.22	PROT
	ATOM	32 CB LEU 204	35.853 25.081 51.353 1.00 30.47	PROT
	ATOM	33 CG LEU 204	35.567 25.083 52.862 1.00 23.17	PROT
	ATOM	34 CD1 LEU 204	35.904 26.439 53.443 1.00 5.41	PROT
25	ATOM	35 CD2 LEU 204	34.106 24.748 53.111 1.00 12.70	PROT
	ATOM	36 C LEU 204	37.424 23.156 51.100 1.00 40.17	PROT
	ATOM	37 O LEU 204	38.219 22.736 51.951 1.00 45.33	PROT
	ATOM	38 N GLN 205	36.682 22.360 50.329 1.00 43.86	PROT
20	ATOM	39 CA GLN 205	36.754 20.899 50.415 1.00 43.96	PROT
30	ATOM	40 CB GLN 205	36.089 20.261 49.184 1.00 45.56	PROT
	ATOM	41 CG GLN 205	34.562 20.195 49.245 1.00 42.39	PROT
	ATOM	42 CD GLN 205	34.022 18.775 49.159 1.00 46.79 33.258 18.444 48.252 1.00 38.84	PROT PROT
	ATOM ATOM	43 OE1 GLN 205 44 NE2 GLN 205	34.412 17.932 50.109 1.00 37.95	PROT
35	ATOM	45 C GLN 205	38.224 20.482 50.483 1.00 42.39	PROT
33	ATOM	46 O GLN 205	38.630 19.702 51.355 1.00 42.39	PROT
	ATOM	47 N LYS 206	39.014 21.015 49.553 1.00 42.37	PROT
	ATOM	48 CA LYS 206	40.440 20.729 49.505 1.00 44.40	PROT
	ATOM	49 CB LYS 206	41.110 21.531 48.385 1.00 38.73	PROT
40	ATOM	50 C LYS 206	41.024 21.118 50.853 1.00 42.36	PROT
	ATOM	51 O LYS 206	41.550 20.271 51.570 1.00 46.93	PROT
	ATOM	52 N SER 207	40.913 22.401 51.192 1.00 34.68	PROT
	ATOM	53 CA SER 207	41.415 22.933 52.455 1.00 29.43	PROT
	ATOM	54 CB SER 207	40,690 24.228 52.791 1.00 24.63	PROT
45	ATOM	55 OG SER 207	41,327 25.332 52.173 1.00 36.56	PROT
	ATOM	56 C SER 207	41.254 21.958 53.614 1.00 29.20	PROT
	ATOM	57 O SER 207	42.223 21.623 54.293 1.00 31.01	PROT
	ATOM		40.028 21.504 53.841 1.00 22.55	PROT
	ATOM	59 CA ILE 208	39.777 20.568 54.928 1.00 27.93	PROT
50	ATOM	60 CB ILE 208	38.267 20.216 55.027 1.00 39.85	PROT

	ATOM	61 CG2 ILE 208	38.062 18.895 55.769 1.00 32.13	PROT
	ATOM	62 CG1 ILE 208	37.528 21.340 55.753 1.00 37.63	PROT
	ATOM	63 CD1 ILE 208	36.788 22.296 54.827 1.00 41.47	PROT
	ATOM	64 C ILE 208	40.591 19.291 54.725 1.00 29.61	PROT
5	ATOM	65 O ILE 208	40.905 18.580 55.679 1.00 40.00	PROT
	ATOM	66 N GLY 209	40.928 19.002 53.475 1.00 35.05	PROT
	ATOM	67 CA GLY 209	41.698 17.809 53.181 1.00 31.94	PROT
	ATOM	68 C GLY 209	40.826 16.695 52.643 1.00 28.66	PROT
	ATOM	69 O GLY 209	41.257 15.553 52.532 1.00 19.46	PROT
10	ATOM	70 N HIS 210	39.586 17.021 52.313 1.00 20.47	PROT
	ATOM	71 CA HIS 210	38.684 16.018 51.774 1.00 26.99	PROT
	ATOM	72 CB HIS 210	37.240 16.451 52.012 1.00 37.16	PROT
	ATOM	73 C HIS 210	38.959 15.806 50.266 1.00 27.75	PROT
	ATOM	74 O HIS 210	39.328 16.741 49.550 1.00 34.08	PROT
15	ATOM	75 N LYS 211	38.807 14.566 49.805 1.00 16.50	PROT
	ATOM	76 CA LYS 211	39.019 14.206 48.403 1.00 5.57	PROT
	ATOM	77 CB LYS 211	39.932 12.981 48.295 1.00 5.67	PROT
	ATOM	78 CG LYS 211	41.370 13.208 48.742 1.00 7.30	PROT
	ATOM	79 CD LYS 211	41.873 14.594 48.347 1.00 14.34	PROT
20	ATOM	80 CE LYS 211	43.339 14.556 47.897 1.00 29.48	PROT
	ATOM	81 NZ LYS 211	43.777 15.851 47.262 1.00 33.43	PROT
	ATOM	82 C LYS 211	37.642 13.861 47.876 1.00 2.73	PROT
	ATOM	83 O LYS 211	37.176 12.741 48.039 1.00 6.57	PROT
	ATOM	84 N PRO 212	36.983 14.813 47.208 1.00 2.00	PROT
25	ATOM	85 CD PRO 212	37.472 16.156 46.846 1.00 10.43	PROT
	ATOM	86 CA PRO 212	35.642 14.542 46.689 1.00 2.05	PROT
	ATOM	87 CB PRO 212	35.088 15.928 46.341 1.00 10.09	PROT
	ATOM	88 CG PRO 212	36.240 16.888 46.422 1.00 8.43	PROT
	ATOM	89 C PRO 212	35.523 13.578 45.520 1.00 2.00	PROT
30	ATOM	90 O PRO 212	36.344 13.554 44.611 1.00 6.04	PROT
	ATOM	91 N GLU 213	34.476 12.773 45.577 1.00 2.68	PROT
	ATOM	92 CA GLU 213	34.181 11.817 44.542 1.00 6.81	PROT
	ATOM	93 CB GLU 213	33.539 10.594 45.173 1.00 7.20	PROT
	ATOM	94 CG GLU 213	34.222 10.232 46.462 1.00 15.33	PROT
35	ATOM	95 CD GLU 213	34.293 8.743 46.689 1.00 21.36	PROT
	ATOM	96 OE1 GLU 213	33.334 8.051 46.290 1.00 29.32	PROT
	ATOM	97 OE2 GLU 213	35.301 8.265 47.268 1.00 28.50	PROT
	ATOM	98 C GLU 213	33.229 12.543 43.584 1.00 12.00	PROT
	ATOM	99 O GLU 213	32.693 13.599 43.926 1.00 19.02	PROT
40	ATOM	100 N PRO 214	33.011 11.985 42.375 1.00 25.74	PROT
	ATOM	101 CD PRO 214	33.592 10.692 41.973 1.00 28.98	PROT
	ATOM	102 CA PRO 214	32.145 12.536 41.322 1.00 23.38	PROT
	ATOM	103 CB PRO 214	32.180 11.476 40.232 1.00 18.01	PROT
	ATOM	104 CG PRO 214	33.376 10.665 40.514 1.00 27.50	PROT
45	ATOM	105 C PRO 214	30.715 12.828 41.734 1.00 25.02	PROT
	ATOM	106 O PRO 214	30.069 11.986 42.355 1.00 31.17	PROT
	ATOM	107 N THR 215	30.211 14.009 41.377 1.00 19.56	PROT
	ATOM	108 CA THR 215	28.830 14.352 41.714 1.00 24.48	PROT
	ATOM	109 CB THR 215	28.535 15.841 41.522 1.00 27.13	PROT
50	ATOM	110 OG1 THR 215	27.939 16.038 40.234 1.00 40.19	PROT

	ATOM	111 CG2 THR 215	29.805 16.659 41.640 1.00 30.81	PROT
	ATOM	112 C THR 215	27.899 13.562 40.805 1.00 22.14	PROT
	ATOM	113 O THR 215	28.357 12.905 39.883 1.00 27.52	PROT
	ATOM	114 N ASP 216	26.599 13.617 41.072 1.00 35.65	PROT
5	ATOM	115 CA ASP 216	25.631 12.890 40.258 1.00 41.16	PROT
	ATOM	116 CB ASP 216	24.219 13.091 40.810 1.00 38.17	PROT
	ATOM	117 C ASP 216	25.714 13.370 38.810 1.00 40.44	PROT
	ATOM	118 O ASP 216	25.683 12.569 37.874 1.00 38.26	PROT
	ATOM	119 N GLU 217	25.832 14.682 38.635 1.00 40.14	PROT
10	ATOM	120 CA GLU 217	25.932 15.275 37.305 1.00 38.89	PROT
	ATOM	121 CB GLU 217	25.883 16.796 37.413 1.00 29.95	PROT
	ATOM	122 C GLU 217	27.231 14.829 36.619 1.00 39.44	PROT
	ATOM	123 O GLU 217	27.245 14.525 35.425 1.00 40.08	PROT
	ATOM	124 N GLU 218	28.319 14.794 37.384 1.00 34.92	PROT
15	ATOM	125 CA GLU 218	29.615 14.370 36.871 1.00 23.70	PROT
	ATOM	126 CB GLU 218	30.698 14.606 37.924 1.00 18.47	PROT
	ATOM	127 CG GLU 218	30.990 16.067 38.198 1.00 15.66	PROT
	ATOM	128 CD GLU 218	32.085 16.264 39.231 1.00 26.88	PROT
	ATOM	129 OE1 GLU 218	32.164 15.458 40.191 1.00 25.07	PROT
20	ATOM	130 OE2 GLU 218	32.864 17.232 39.078 1.00 33.79	PROT
	ATOM	131 C GLU 218	29.589 12.892 36.491 1.00 21.05	PROT
	ATOM	132 O GLU 218	30.182 12.490 35.495 1.00 24.30	PROT
	ATOM	133 N TRP 219	28.907 12.080 37.288 1.00 13.98	PROT
	ATOM	134 CA TRP 219	28.829 10.660 37.000 1.00 17.30	PROT
25	ATOM	135 CB TRP 219	28.052 9.921 38.089 1.00 16.27	PROT
	ATOM	136 CG TRP 219	28.890 9.520 39.277 1.00 31.14	PROT
	ATOM	137 CD2 TRP 219	29.984 8.585 39.296 1.00 36.40	PROT
	ATOM	138 CE2 TRP 219	30.476 8.547 40.621 1.00 29.24	PROT
	ATOM	139 CE3 TRP 219	30.595 7.781 38.323 1.00 41.61	PROT
30	ATOM	140 CD1 TRP 219	28.771 9.988 40.551 1.00 28.69	PROT
	ATOM	141 NE1 TRP 219	29.718 9.411 41.362 1.00 35.01	PROT
	ATOM	142 CZ2 TRP 219	31.552 7.737 41.004 1.00 30.89	PROT
	ATOM	143 CZ3 TRP 219	31.673 6.969 38.707 1.00 45.72	PROT
	ATOM	144 CH2 TRP 219	32.137 6.958 40.038 1.00 35.17	PROT
35	ATOM	145 C TRP 219	28.125 10.500 35.660 1.00 20.83	PROT
	ATOM	146 O TRP 219	28.467 9.616 34.865 1.00 31.36	PROT
	ATOM	147 N GLU 220	27.143 11.364 35.412 1.00 30.53	PROT
	ATOM	148 CA GLU 220	26.400 11.323 34.159 1.00 33.95	PROT
	ATOM	149 CB GLU 220	25.237 12.318 34.201 1.00 22.17	PROT
40	ATOM	150 C GLU 220	27.356 11.658 33.013 1.00 34.66	PROT
	ATOM	151 O GLU 220	27.233 11.134 31.900 1.00 43.86	PROT
	ATOM	152 N LEU 221	28.320 12.528 33.297 1.00 22.60	PROT
	ATOM	153 CA LEU 221	29.305 12.926 32.304 1.00 17.18	PROT
	ATOM	154 CB LEU 221	29.995 14.219 32.743 1.00 11.03	PROT
45	ATOM	155 CG LEU 221	31.078 14.824 31.850 1.00 5.17	PROT PROT
	ATOM	156 CD1 LEU 221	30.756 14.569 30.415 1.00 6.41	
	ATOM	157 CD2 LEU 221	31.181 16.305 32.092 1.00 10.65	PROT PROT
	ATOM	158 C LEU 221	30.344 11.817 32.122 1.00 22.25 30.759 11.521 31.002 1.00 18.99	PROT
50	ATOM	159 O LEU 221		PROT
50	ATOM	160 N ILE 222	30.754 11.198 33.228 1.00 20.74	FKUI

	ATOM	161 CA ILE 222 31.744 10.136 33.177 1.00 12.88	PROT
	ATOM	162 CB ILE 222 32.115 9.662 34.587 1.00 12.96	PROT
	ATOM	163 CG2 ILE 222 33.030 8.468 34.515 1.00 2.00	PROT
	ATOM	164 CG1 ILE 222 32.811 10.796 35.332 1.00 16.50	PROT
5	ATOM	165 CD1 ILE 222 33.625 10.351 36.511 1.00 15.90	PROT
	ATOM		PROT
	ATOM		PROT
	ATOM	168 N LYS 223 29.966 8.618 32.530 1.00 33.88	PROT
	ATOM	169 CA LYS 223 29.371 7.503 31.795 1.00 39.02	PROT
10	ATOM	170 CB LYS 223 27.908 7.307 32.224 1.00 40.29	PROT
	ATOM	171 C LYS 223 29.444 7.779 30.293 1.00 39.14	PROT
	ATOM	172 O LYS 223 29.949 6.963 29.517 1.00 32.99	PROT
	ATOM	173 N THR 224 28.936 8.942 29.897 1.00 27.19	PROT
	ATOM	174 CA THR 224 28.929 9.363 28.498 1.00 25.75	PROT
15	ATOM	175 CB THR 224 28.440 10.817 28.407 1.00 22.51	PROT
	ATOM	176 OG1 THR 224 27.018 10.837 28.568 1.00 35.46	
	ATOM	177 CG2 THR 224 28.799 11.436 27.083 1.00 15.53	PROT
	ATOM	178 C THR 224 30.307 9.235 27.833 1.00 22.31	PROT
	ATOM	179 O THR 224 30.480 8.517 26.843 1.00 27.13	PROT
20	ATOM	180 N VAL 225 31.287 9.936 28.386 1.00 17.87	PROT
	ATOM	181 CA VAL 225 32.635 9.906 27.854 1.00 17.07	PROT
	ATOM	182 CB VAL 225 33.559 10.759 28.720 1.00 16.86	PROT
	ATOM	183 CG1 VAL 225 34.845 11.064 27.973 1.00 26.54	
	ATOM	184 CG2 VAL 225 32.854 12.057 29.075 1.00 24.46	
25	ATOM	185 C VAL 225 33.169 8.486 27.793 1.00 16.11	PROT
	ATOM	186 O VAL 225 33.683 8.042 26.763 1.00 12.75	PROT
	ATOM	187 N THR 226 33.040 7.769 28.900 1.00 12.23	PROT
	ATOM	188 CA THR 226 33.520 6.400 28.951 1.00 12.34	PROT
	ATOM	189 CB THR 226 33.175 5.747 30.271 1.00 17.01	PROT
30	ATOM	190 OG1 THR 226 33.715 6.536 31.342 1.00 6.78	PROT
	ATOM	191 CG2 THR 226 33.739 4.324 30.307 1.00 2.00	PROT
	ATOM	192 C THR 226 32.909 5.581 27.837 1.00 14.82	PROT
	ATOM	193 O THR 226 33.623 4.953 27.061 1.00 20.90	PROT
	ATOM	194 N GLU 227 31.582 5.588 27.758 1.00 22.90	PROT
35	ATOM	195 CA GLU 227 30.886 4.849 26.714 1.00 22.63	PROT
	ATOM	196 CB GLU 227 29.417 5.248 26.678 1.00 20.14	PROT
	ATOM	197 C GLU 227 31.556 5.173 25.386 1.00 21.74	PROT
	ATOM	198 O GLU 227 32.057 4.283 24.700 1.00 24.42	PROT
	ATOM	199 N ALA 228 31.590 6.460 25.050 1.00 13.26	PROT
40	ATOM	200 CA ALA 228 32.196 6.928 23.800 1.00 22.76	PROT
	ATOM	201 CB ALA 228 32.267 8.450 23.785 1.00 22.50	PROT
	ATOM	202 C ALA 228 33.584 6.358 23.538 1.00 19.19	PROT
	ATOM	203 O ALA 228 33.913 6.003 22.408 1.00 17.19	PROT
	ATOM	204 N HIS 229 34.408 6.290 24.573 1.00 20.11	PROT
45	ATOM	205 CA HIS 229 35.741 5.756 24.389 1.00 18.68	PROT
	ATOM	206 CB HIS 229 36.537 5.819 25.686 1.00 10.37	PROT
	ATOM	207 CG HIS 229 37.894 5.201 25.586 1.00 2.00	PROT
	ATOM	208 CD2 HIS 229 38.524 4.299 26.376 1.00 7.61	PROT
	ATOM	209 ND1 HIS 229 38.780 5.517 24.582 1.00 3.78	PROT
50	ATOM	210 CE1 HIS 229 39.900 4.837 24.758 1.00 15.67	PROT

	ATOM	211 NE2 HIS 229	39.771 4.090 25.840 1.00 7.10	PROT
	ATOM			PROT
	ATOM		36.127 3.950 22.866 1.00 22.42	PROT
	ATOM	214 N VAL 230	34.983 3.505 24.762 1.00 21.64	PROT
5	ATOM	215 CA VAL 230	34.827 2.086 24.468 1.00 33.80	PROT
J	ATOM	216 CB VAL 230	33.960 1.388 25.528 1.00 33.11	PROT
	ATOM	217 CG1 VAL 230	34.251 -0.106 25.515 1.00 33.80	PROT
	ATOM	218 CG2 VAL 230	34.228 1.985 26.896 1.00 26.54	PROT
	ATOM	219 C VAL 230	34.224 1.781 23.100 1.00 33.12	PROT
10	ATOM	220 O VAL 230	34.703 0.897 22.385 1.00 40.80	PROT
10	ATOM	221 N ALA 231	33.170 2.507 22.746 1.00 36.22	PROT
	ATOM	222 CA ALA 231	32.497 2.298 21.471 1.00 36.24	PROT
	ATOM	223 CB ALA 231	31.318 3.255 21.343 1.00 18.90	PROT
	ATOM	224 C ALA 231	33.445 2.501 20.303 1.00 37.54	PROT
15	ATOM	225 O ALA 231	33.342 1.816 19.285 1.00 35.93	PROT
13	ATOM	226 N THR 232	34.380 3.434 20.474 1.00 23.74	PROT
	ATOM	227 CA THR 232	35.329 3.789 19.432 1.00 15.54	PROT
	ATOM	228 CB THR 232	35.335 5.321 19.238 1.00 9.70	PROT
	ATOM	229 OG1 THR 232	35.733 5.949 20.460 1.00 16.73	PROT
20	ATOM	230 CG2 THR 232	33.942 5.828 18.891 1.00 2.00	PROT
20	ATOM	231 C THR 232	36.758 3.309 19.670 1.00 19.86	PROT
	ATOM	232 O THR 232	37.695 3.854 19.094 1.00 15.31	PROT
	ATOM	232 O THR 232 233 N ASN 233	36.938 2.305 20.523 1.00 28.26	PROT
	ATOM	234 CA ASN 233	38.280 1.771 20.772 1.00 39.32	PROT
25	ATOM	235 CB ASN 233	38.435 1.343 22.234 1.00 47.14	PROT
23	ATOM	236 CG ASN 233	39.804 1.689 22.801 1.00 54.02	PROT
	ATOM	237 OD1 ASN 233	40.633 2.303 22.128 1.00 60.36	PROT
	ATOM	238 ND2 ASN 233	40.045 1.296 24.045 1.00 48.67	PROT
	ATOM	239 C ASN 233	38.507 0.574 19.840 1.00 49.33	PROT
30	ATOM	240 O ASN 233	38.338 0.693 18.625 1.00 65.36	PROT
50	ATOM	241 N ALA 234	38.877 -0.577 20.388 1.00 57.89	PROT
	ATOM	242 CA ALA 234	39.090 -1.752 19.552 1.00 57.22	PROT
	ATOM	243 CB ALA 234	40.372 -1.595 18.754 1.00 48.03	PROT
	ATOM	244 C ALA 234	39.141 -3.027 20.384 1.00 62.42	PROT
35	ATOM	245 O ALA 234	38.471 -3.073 21.440 1.00 56.93	PROT
55	ATOM	246 OT ALA 234	39.853 -3.968 19.965 1.00 76.16	PROT
	ATOM	247 N TRP 239	41.987 -7.449 22.970 1.00 58.82	PROT
	ATOM	248 CA TRP 239	43.077 -6.886 22.154 1.00 51.37	PROT
	ATOM	249 CB TRP 239	43.325 -5.406 22.534 1.00 45.12	PROT
40	ATOM	250 CG TRP 239	44.193 -5.170 23.760 1.00 43.09	PROT
	ATOM	251 CD2 TRP 239	45.617 -5.037 23.793 1.00 32.36	PROT
	ATOM	252 CE2 TRP 239	45.990 -4.872 25.142 1.00 28.37	PROT
	ATOM	253 CE3 TRP 239	46.615 -5.049 22.813 1.00 40.79	PROT
	ATOM	254 CD1 TRP 239	43.773 -5.073 25.059 1.00 46.63	PROT
45	ATOM	255 NE1 TRP 239	44.847 -4.896 25.893 1.00 27.08	PROT
	ATOM	256 CZ2 TRP 239	47.315 -4.717 25.535 1.00 35.48	PROT
	ATOM	257 CZ3 TRP 239	47.936 -4.896 23.204 1.00 40.18	PROT
	ATOM	258 CH2 TRP 239	48.273 -4.733 24.554 1.00 49.93	PROT
	ATOM	259 C TRP 239	44.422 -7.623 22.063 1.00 49.76	PROT
50	ATOM	260 O TRP 239	44.944 -7.799 20.962 1.00 48.14	PROT
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ATOM
             261 N LYS 240
                               44.975 -8.048 23.198 1.00 38.92
                                                              PROT
     ATOM
             262 CA LYS 240
                                46.263 -8.735 23.232 1.00 37.29
                                                               PROT
     ATOM
             263 CB LYS 240
                                46.572 -9.196 24.657 1.00 38.79
                                                               PROT
     ATOM
             264 CG LYS 240
                                47.106 -8.099 25.571 1.00 38.43
                                                               PROT
     ATOM
             265 CD LYS 240
                                48.307 -8.584 26.370 1.00 35.71
                                                               PROT
     ATOM
             266 CE LYS 240
                                48.631 -7.646 27.523 1.00 37.87
                                                               PROT
                                                               PROT
     ATOM
             267 NZ LYS 240
                                49.058 -8.377 28.750 1.00 28.85
                               46.404 -9.914 22.269 1.00 42.18
                                                              PROT
     ATOM
             268 C LYS 240
             269 O LYS 240
                               47.491 -10.132 21.732 1.00 45.89
                                                              PROT
     ATOM
             270 N GLN 241
                               45.331 -10.679 22.058 1.00 46.08
                                                               PROT
10
     ATOM
             271 CA GLN 241
                                45.390 -11.816 21.133 1.00 45.02
                                                               PROT
     ATOM
            272 CB GLN 241
                                44.575 -13.011 21.638 1.00 46.30
                                                               PROT
     ATOM
                                                               PROT
            273 CG GLN 241
                                44.284 -13.018 23.116 1.00 60.38
     ATOM
     ATOM
            274 CD GLN 241
                                42.828 -13.312 23.408 1.00 63.76
                                                               PROT
     ATOM
             275 OE1 GLN 241
                                42.154 -13.988 22.631 1.00 66.34
                                                                PROT
15
             276 NE2 GLN 241
                                 42.333 -12.801 24.531 1.00 69.18
                                                                PROT
     ATOM
     ATOM
             277 C GLN 241
                               44.866 -11.405 19.764 1.00 45.77
                                                               PROT
     ATOM
             278 O GLN 241
                               45.107 -12.085 18.765 1.00 51.18
                                                               PROT
             279 N LYS 242
     ATOM
                               44.132 -10.300 19.723 1.00 42.04
                                                              PROT
             280 CA LYS 242
20
                                43.613 -9.794 18.464 1.00 48.33
                                                               PROT
     ATOM
             281 CB LYS 242
                                42.498 -8.786 18.727 1.00 40.17
     ATOM
                                                               PROT
             282 C LYS 242
                               44.796 -9.123 17.742 1.00 53.04
                                                              PROT
     ATOM
             283 O LYS 242
                               44.709 -8.753 16.565 1.00 48.21
                                                              PROT
     ATOM
             284 N ARG 243
                               45.906 -8.992 18.470 1.00 45.44
     ATOM
                                                              PROT
             285 CA ARG 243
                                47.128 -8.374 17.965 1.00 43.53
                                                               PROT
25
     ATOM
                                48.108 -8.135 19.118 1.00 40.21
            286 CB ARG 243
                                                               PROT
     ATOM
            287 C ARG 243
                               47.795 -9.220 16.892 1.00 45.96
     ATOM
                                                              PROT
     ATOM
            288 O ARG 243
                               47.684 -10.443 16.894 1.00 50.22
                                                               PROT
     ATOM
             289 N LYS 244
                               48.498 -8.551 15.982 1.00 52.12
                                                              PROT
30
     ATOM
             290 CA LYS 244
                                49.202 -9.202 14.879 1.00 45.30
                                                               PROT
             291 CB LYS 244
                                48.466 -8.950 13.558 1.00 48.24
     ATOM
                                                               PROT
             292 CG LYS 244
     ATOM
                                47.109 -9.631 13.446 1.00 53.78
                                                               PROT
            293 CD LYS 244
     ATOM
                                46.835 -10.078 12.011 1.00 60.50
                                                               PROT
     ATOM
            294 CE LYS 244
                                46.038 -9.030 11.241 1.00 61.03
                                                              PROT
35
     ATOM
             295 NZ LYS 244
                               45.455 -7.997 12.146 1.00 55.25
                                                              PROT
            296 C LYS 244
                               50.616 -8.641 14.786 1.00 40.33
     ATOM
                                                              PROT
            297 O LYS 244
                               50.849 -7.629 14.125 1.00 36.07
                                                              PROT
     ATOM
            298 N PHE 245
                               51.556 -9.312 15.445 1.00 27.87
     ATOM
                                                              PROT
     ATOM
            299 CA PHE 245
                                52.949 -8.885 15.461 1.00 30.61
                                                              PROT
40
     ATOM
            300 CB PHE 245
                                53.784 -9.887 16.253 1.00 20.28
                                                              PROT
     ATOM
            301 CG PHE 245
                                53.454 -9.922 17.713 1.00 37.23
                                                               PROT
     ATOM
             302 CD1 PHE 245
                                52.636 -10.917 18.234 1.00 40.93
                                                               PROT
     ATOM
            303 CD2 PHE 245
                                53.958 -8.959 18.577 1.00 41.60
                                                               PROT
             304 CE1 PHE 245
                                52.326 -10.953 19.594 1.00 42.54
                                                               PROT
     ATOM
             305 CE2 PHE 245
                                53.652 -8.989 19.936 1.00 45.84
45
     ATOM
                                                               PROT
            306 CZ PHE 245
                               52.835 -9.988 20.443 1.00 33.72
     ATOM
                                                              PROT
                               53.549 -8.693 14.068 1.00 38.75
            307 C PHE 245
     ATOM
                                                              PROT
                               53.794 -9.660 13.337 1.00 48.93
     ATOM
             308 O PHE 245
                                                              PROT
     ATOM
            309 N LEU 246
                               53.789 -7.437 13.704 1.00 41.18
                                                              PROT
50
     ATOM
            310 CA LEU 246
                               54.362 -7.124 12.404 1.00 43.43
                                                              PROT
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	ATOM	311 CB LEU 246 54.378 -5.612 12.181 1.00 42.78 PROT	
	ATOM	312 CG LEU 246 54.535 -5.200 10.718 1.00 49.88 PROT	
	ATOM	313 CD1 LEU 246 53.528 -4.113 10.365 1.00 40.64 PROT	
_	ATOM	314 CD2 LEU 246 55.966 -4.730 10.485 1.00 48.66 PROT	
5	ATOM	315 C LEU 246 55.777 -7.692 12.250 1.00 42.60 PROT	
	ATOM	316 O LEU 246 56.677 -7.383 13.028 1.00 45.75 PROT	
	ATOM	317 N PRO 247 55.977 -8.540 11.233 1.00 50.03 PROT	
	ATOM	318 CD PRO 247 54.914 -8.924 10.286 1.00 60.17 PROT	
	ATOM	319 CA PRO 247 57.237 -9.199 10.894 1.00 49.90 PROT	
10	ATOM	320 CB PRO 247 57.181 -9.282 9.369 1.00 59.51 PROT	
	ATOM	321 CG PRO 247 55.678 -9.244 9.023 1.00 52.86 PROT	
	ATOM	322 C PRO 247 58.499 -8.494 11.392 1.00 48.85 PROT	
	ATOM	323 O PRO 247 58.675 -7.295 11.186 1.00 49.28 PROT	
	ATOM	324 N GLU 248 59.379 -9.261 12.032 1.00 47.62 PROT	
15	ATOM	325 CA GLU 248 60.628 -8.733 12.574 1.00 51.41 PROT	
	ATOM	326 CB GLU 248 61.266 -9.750 13.522 1.00 44.22 PROT	
	ATOM	327 C GLU 248 61.623 -8.354 11.490 1.00 53.28 PROT	
	ATOM	328 O GLU 248 62.815 -8.214 11.765 1.00 62.57 PROT	
	ATOM	329 N ASP 249 61.146 -8.200 10.258 1.00 56.20 PROT	
20	ATOM	330 CA ASP 249 62.030 -7.818 9.164 1.00 55.88 PROT	
	ATOM	331 CB ASP 249 62.231 -8.981 8.173 1.00 53.88 PROT	
	ATOM	332 CG ASP 249 60.928 -9.637 7.739 1.00 54.39 PROT	
	ATOM	333 OD1 ASP 249 60.578 -10.693 8.310 1.00 57.70 PROT	
	ATOM	334 OD2 ASP 249 60.264 -9.112 6.819 1.00 45.76 PROT	
25	ATOM	335 C ASP 249 61.539 -6.567 8.437 1.00 54.20 PROT	
	ATOM	336 O ASP 249 62.119 -6.154 7.429 1.00 55.31 PROT	
	ATOM	337 N ILE 250 60.469 -5.965 8.954 1.00 46.13 PROT	
	ATOM	338 CA ILE 250 59.933 -4.735 8.376 1.00 46.12 PROT	
- ^	ATOM	339 CB ILE 250 58.413 -4.764 8.253 1.00 43.38 PROT	
30	ATOM	340 CG2 ILE 250 57.892 -3.344 8.057 1.00 39.15 PROT	
	ATOM	341 CG1 ILE 250 58.007 -5.654 7.074 1.00 48.96 PROT	
	ATOM	342 CD1 ILE 250 56.707 -6.401 7.283 1.00 43.14 PROT	
	ATOM	343 C ILE 250 60.311 -3.590 9.294 1.00 45.32 PROT	
	ATOM	344 O ILE 250 60.257 -3.724 10.513 1.00 43.74 PROT	
35	ATOM	345 N GLY 251 60.680 -2.459 8.711 1.00 36.80 PROT	
	ATOM	346 CA GLY 251 61.091 -1.329 9.521 1.00 39.28 PROT	
	ATOM	347 C GLY 251 62.370 -1.621 10.305 1.00 44.31 PROT	
	ATOM	348 O GLY 251 62.538 -1.145 11.428 1.00 51.39 PROT	
	ATOM	349 N GLN 252 63.277 -2.399 9.715 1.00 55.47 PROT	
40	ATOM	350 CA GLN 252 64.536 -2.745 10.374 1.00 54.24 PROT	
	ATOM	351 CB GLN 252 64.792 -4.237 10.245 1.00 49.31 PROT	
	ATOM	352 C GLN 252 65.720 -1.959 9.812 1.00 54.86 PROT	
	ATOM	353 O GLN 252 65.492 -1.079 8.953 1.00 58.80 PROT	
	ATOM	354 CB VAL 264 60.887 6.759 5.510 1.00 34.33 PROT	
45	ATOM	355 CG1 VAL 264 59.550 6.086 5.790 1.00 34.34 PROT	
	ATOM	356 CG2 VAL 264 60.893 8.163 6.080 1.00 20.22 PROT	
	ATOM	357 C VAL 264 62.053 4.557 5.439 1.00 34.08 PROT	
	ATOM	358 O VAL 264 62.280 4.466 4.232 1.00 46.39 PROT	
	ATOM	359 N VAL 264 63.361 6.605 5.966 1.00 21.27 PROT	
50	ATOM	360 CA VAL 264 62.041 5.920 6.122 1.00 29.68 PROT	

	ATOM	361 N ASP 265	61.809 3.499 6.209 1.00 40.63	PROT
	ATOM	362 CA ASP 265	61.796 2.141 5.670 1.00 43.58	PROT
	ATOM	363 CB ASP 265	61.243 1.160 6.704 1.00 44.07	PROT
	ATOM	364 CG ASP 265	61.179 -0.262 6.185 1.00 49.19	PROT
5	ATOM	365 OD1 ASP 265	62.223 -0.945 6.175 1.00 57.67	PROT
	ATOM	366 OD2 ASP 265	60.082 -0.702 5.789 1.00 54.75	PROT
	ATOM	367 C ASP 265	60.956 2.071 4.401 1.00 48.03	PROT
	ATOM	368 O ASP 265	61.362 1.458 3.411 1.00 57.44	PROT
	ATOM	369 N LEU 266	59.793 2.711 4.436 1.00 40.55	PROT
10	ATOM	370 CA LEU 266	58.879 2.741 3.295 1.00 45.78	PROT
	ATOM	371 CB LEU 266	59.638 2.962 1.977 1.00 45.92	PROT
	ATOM	372 CG LEU 266	59.881 4.407 1.506 1.00 48.41	PROT
	ATOM	373 CD1 LEU 266	59.934 4.432 -0.007 1.00 32.83	PROT
	ATOM	374 CD2 LEU 266	58.787 5.344 2.012 1.00 45.08	PROT
15	ATOM	375 C LEU 266	58.064 1.462 3.214 1.00 45.45	PROT
	ATOM	376 O LEU 266	56.862 1.503 2.949 1.00 42.92	PROT
	ATOM	377 N GLU 267	58.712 0.324 3.431 1.00 46.47	PROT
	ATOM	378 CA GLU 267	57.986 -0.935 3.415 1.00 44.34	PROT
	ATOM	379 CB GLU 267	58.943 -2.123 3.505 1.00 39.42	PROT
20	ATOM	380 CG GLU 267	58.291 -3.457 3.188 1.00 40.68	PROT
	ATOM	381 CD GLU 267	58.929 -4.607 3.943 1.00 63.54	PROT
	ATOM	382 OE1 GLU 267	60.103 -4.470 4.361 1.00 68.92	PROT
	ATOM	383 OE2 GLU 267	58.258 -5.650 4.120 1.00 66.66	PROT
	ATOM	384 C GLU 267	57.106 -0.880 4.655 1.00 41.57	PROT
25	ATOM	385 O GLU 267	55.991 -1.398 4.673 1.00 48.68	PROT
	ATOM	386 N ALA 268	57.620 -0.215 5.686 1.00 39.33	PROT
	ATOM	387 CA ALA 268	56.916 -0.057 6.951 1.00 31.62	PROT
	ATOM	388 CB ALA 268	57.918 0.134 8.063 1.00 7.56	PROT
	ATOM	389 C ALA 268	55.960 1.135 6.888 1.00 25.96	PROT
30	ATOM	390 O ALA 268	54.786 1.036 7.237 1.00 17.35	PROT
	ATOM	391 N PHE 269	56.464 2.274 6.446 1.00 11.34	PROT
	ATOM	392 CA PHE 269	55.615 3.453 6.335 1.00 15.72	PROT
	ATOM	393 CB PHE 269	56.274 4.474 5.405 1.00 20.08	PROT
2.5	ATOM	394 CG PHE 269	55.552 5.788 5.334 1.00 24.67	PROT
35	ATOM	395 CD1 PHE 269	55.661 6.713 6.369 1.00 15.69	PROT
	ATOM	396 CD2 PHE 269	54.772 6.111 4.222 1.00 20.64	PROT
	ATOM	397 CE1 PHE 269	55.003 7.942 6.300 1.00 22.55	PROT
	ATOM	398 CE2 PHE 269 399 CZ PHE 269	54.108 7.342 4.143 1.00 19.77 54.224 8.257 5.186 1.00 19.27	PROT
40	ATOM			PROT
40	ATOM			PROT
	ATOM ATOM	401 O PHE 269 402 N SER 270	53.212 3.351 6.261 1.00 13.40 54.367 2.214 4.692 1.00 43.85	PROT PROT
		402 N SER 270 403 CA SER 270	54.367 2.214 4.692 1.00 43.85 53.217 1.686 3.967 1.00 46.67	PROT
	ATOM ATOM	403 CA SER 270 404 CB SER 270	53.687 0.669 2.924 1.00 53.60	PROT
45	ATOM	404 CB SER 270 405 OG SER 270	52.662 0.382 1.988 1.00 68.82	PROT
43	ATOM	406 C SER 270	52.181 1.039 4.865 1.00 43.32	PROT
	ATOM	400 C SER 270 407 O SER 270	51.024 1.459 4.893 1.00 43.87	PROT
	ATOM	407 O SER 270 408 N HIS 271	52.594 0.009 5.590 1.00 34.59	PROT
	ATOM	409 CA HIS 271	51.681 -0.694 6.486 1.00 37.12	PROT
50	ATOM	410 CB HIS 271	52.441 -1.772 7.266 1.00 46.61	PROT
50		05 116 2/1	32 1	11.01

	ATOM	411 CG HIS 271 52.603 -3.056 6.512 1.00 63.99	PROT
	ATOM	412 CD2 HIS 271 51.879 -4.201 6.533 1.00 62.06	PROT
	ATOM	413 ND1 HIS 271 53.608 -3.256 5.590 1.00 60.86	PROT
	ATOM	414 CE1 HIS 271 53.497 -4.467 5.075 1.00 60.70	PROT
5	ATOM	415 NE2 HIS 271 52.456 -5.061 5.630 1.00 64.10	PROT
	ATOM		PROT
	ATOM	417 O HIS 271 49.744 0.245 7.586 1.00 37.75	PROT
	ATOM	418 N PHE 272 51.752 1.099 8.133 1.00 32.81	PROT
	ATOM	419 CA PHE 272 51.190 2.038 9.085 1.00 27.77	PROT
10	ATOM	420 CB PHE 272 52.302 2.886 9.714 1.00 10.49	PROT
	ATOM	421 CG PHE 272 53.338 2.086 10.459 1.00 6.98	PROT
	ATOM	422 CD1 PHE 272 54.671 2.478 10.449 1.00 4.13	PROT
	ATOM	423 CD2 PHE 272 52.978 0.961 11.193 1.00 6.95	PROT
	ATOM	424 CE1 PHE 272 55.634 1.764 11.163 1.00 7.86	PROT
15	ATOM	425 CE2 PHE 272 53.930 0.242 11.909 1.00 6.13	PROT
13	ATOM	426 CZ PHE 272 55.263 0.645 11.895 1.00 8.93	PROT
	ATOM	427 C PHE 272 50.168 2.939 8.405 1.00 30.96	PROT
	ATOM	428 O PHE 272 49.071 3.156 8.931 1.00 30.21	PROT
	ATOM	429 N THR 273 50.522 3.452 7.231 1.00 31.55	PROT
20	ATOM	430 CA THR 273 49.633 4.343 6.487 1.00 33.39	PROT
20	ATOM	431 CB THR 273 50.335 4.912 5.243 1.00 36.80	PROT
	ATOM	432 OG1 THR 273 50.649 3.847 4.332 1.00 27.42	PROT
	ATOM	433 CG2 THR 273 51.613 5.641 5.656 1.00 32.25	PROT
	ATOM	434 C THR 273 48.350 3.647 6.056 1.00 34.07	PROT
25	ATOM	435 O THR 273 47.362 4.294 5.697 1.00 17.11	PROT
	ATOM	436 N LYS 274 48.372 2.321 6.088 1.00 34.47	PROT
	ATOM	437 CA LYS 274 47.196 1.555 5.726 1.00 42.17	PROT
	ATOM	438 CB LYS 274 47.544 0.069 5.615 1.00 40.02	PROT
	ATOM	439 C LYS 274 46.153 1.778 6.818 1.00 41.47	PROT
30	ATOM	440 O LYS 274 45.115 2.402 6.584 1.00 47.37	PROT
	ATOM		PROT
	ATOM	442 CA ILE 275 45.559 1.403 9.166 1.00 25.49	PROT
	ATOM	443 CB ILE 275 45.991 0.435 10.262 1.00 19.72	PROT
	ATOM	444 CG2 ILE 275 46.290 -0.934 9.642 1.00 23.39	PROT
35	ATOM	445 CG1 ILE 275 47.249 0.958 10.953 1.00 12.96	PROT
	ATOM	446 CD1 ILE 275 47.970 -0.103 11.769 1.00 11.07	PROT
	ATOM		PROT
	ATOM	448 O ILE 275 44.541 3.081 10.547 1.00 18.98	PROT
	ATOM	449 N ILE 276 46.347 3.694 9.402 1.00 8.88	PROT
40	ATOM	450 CA ILE 276 46.268 5.043 9.924 1.00 6.62	PROT
	ATOM	451 CB ILE 276 47.298 5.972 9.261 1.00 21.77	PROT
	ATOM	452 CG2 ILE 276 46.894 6.267 7.831 1.00 27.28	PROT
	ATOM	453 CG1 ILE 276 47.374 7.288 10.028 1.00 6.75	PROT
	ATOM	454 CD1 ILE 276 48.349 7.255 11.153 1.00 15.44	PROT
45	ATOM		PROT
	ATOM	456 O ILE 276 44.349 6.331 10.565 1.00 29.36	PROT
	ATOM	457 N THR 277 44.303 5.411 8.535 1.00 22.12	PROT
	ATOM	458 CA THR 277 43.007 6.005 8.260 1.00 27.16	PROT
	ATOM	459 CB THR 277 42.532 5.675 6.834 1.00 27.11	PROT
50	ATOM	460 OG1 THR 277 43.665 5.584 5.955 1.00 22.55	PROT

	ATOM	461 CG2 THR 277 41.594 6.763 6.337 1.00 26.98 PRO	Т
	ATOM	462 C THR 277 41.944 5.591 9.270 1.00 25.23 PROT	
	ATOM	463 O THR 277 41.271 6.443 9.847 1.00 21.62 PROT	
	ATOM	464 N PRO 278 41.769 4.279 9.491 1.00 18.64 PROT	
5	ATOM	465 CD PRO 278 42.472 3.167 8.832 1.00 9.52 PROT	
_	ATOM	466 CA PRO 278 40.765 3.803 10.453 1.00 18.48 PRO	
	ATOM	467 CB PRO 278 40.907 2.280 10.415 1.00 14.77 PRO	
	ATOM	468 CG PRO 278 42.195 2.008 9.738 1.00 7.70 PROT	
	ATOM	469 C PRO 278 40.956 4.356 11.870 1.00 25.40 PROT	
10	ATOM	470 O PRO 278 39.983 4.628 12.576 1.00 22.33 PROT	
	ATOM	471 N ALA 279 42.211 4.507 12.285 1.00 22.14 PROT	7
	ATOM	472 CA ALA 279 42.519 5.038 13.607 1.00 20.26 PRO	T
	ATOM	473 CB ALA 279 44.016 5.033 13.831 1.00 13.33 PRO	T
	ATOM	474 C ALA 279 41.984 6.456 13.699 1.00 16.49 PROT	
15	ATOM	475 O ALA 279 41.222 6.797 14.598 1.00 32.38 PROT	r
	ATOM	476 N ILE 280 42.384 7.286 12.753 1.00 7.56 PROT	
	ATOM	477 CA ILE 280 41.935 8.666 12.734 1.00 9.96 PROT	
	ATOM	478 CB ILE 280 42.422 9.380 11.462 1.00 8.46 PROT	
	ATOM	479 CG2 ILE 280 42.172 10.871 11.581 1.00 2.00 PRO	Γ
20	ATOM	480 CG1 ILE 280 43.901 9.059 11.220 1.00 10.96 PRO	Γ
	ATOM	481 CD1 ILE 280 44.615 10.036 10.294 1.00 8.54 PRO	Γ
	ATOM	482 C ILE 280 40.410 8.805 12.805 1.00 15.46 PROT	
	ATOM	483 O ILE 280 39.887 9.741 13.421 1.00 24.39 PROT	
	ATOM	484 N THR 281 39.692 7.883 12.172 1.00 24.18 PROT	
25	ATOM	485 CA THR 281 38.238 7.962 12.153 1.00 24.77 PRO	
	ATOM	486 CB THR 281 37.650 6.952 11.145 1.00 33.90 PRO	
	ATOM	487 OG1 THR 281 38.607 6.711 10.108 1.00 34.62 PRO	
	ATOM	488 CG2 THR 281 36.379 7.506 10.513 1.00 39.80 PRC	
	ATOM	489 C THR 281 37.655 7.726 13.535 1.00 23.39 PROT	
30	ATOM	490 O THR 281 36.733 8.422 13.960 1.00 19.51 PROT	
	ATOM	491 N ARG 282 38.213 6.743 14.234 1.00 16.90 PROT	
	ATOM	492 CA ARG 282 37.781 6.404 15.583 1.00 12.29 PRO	
	ATOM	493 CB ARG 282 38.641 5.260 16.115 1.00 5.36 PRO	
	ATOM	494 CG ARG 282 37.936 3.926 16.136 1.00 17.05 PRO	
35	ATOM	495 CD ARG 282 38.296 3.095 14.942 1.00 18.41 PRO	
	ATOM	496 NE ARG 282 39.622 2.475 15.011 1.00 35.77 PRO	
	ATOM	497 CZ ARG 282 40.454 2.501 16.055 1.00 36.80 PRO 498 NH1 ARG 282 41.629 1.888 15.967 1.00 35.96 PRO	
	ATOM		
40	ATOM		
40	ATOM		
	ATOM ATOM	501 O ARG 282 37.078 7.758 17.456 1.00 22.98 PROT 502 N VAL 283 38.813 8.518 16.268 1.00 11.92 PROT	
	ATOM	503 CA VAL 283 38.937 9.719 17.083 1.00 14.68 PRO	
	ATOM	504 CB VAL 283 40.191 10.541 16.696 1.00 23.35 PRO	
45	ATOM	505 CG1 VAL 283 40.467 11.593 17.752 1.00 11.98 PRO	
73	ATOM	506 CG2 VAL 283 41.396 9.621 16.526 1.00 20.41 PRO	
	ATOM	507 C VAL 283 37.705 10.580 16.833 1.00 12.72 PRO	
	ATOM	508 O VAL 283 36.965 10.929 17.752 1.00 20.37 PRO	
	ATOM	509 N VAL 284 37.503 10.920 15.567 1.00 18.28 PRO	
50	ATOM	510 CA VAL 284 36.369 11.727 15.150 1.00 16.98 PRO	
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PROT
     ATOM
            511 CB VAL 284
                               36.251 11.765 13.602 1.00 27.40
                               35.434 12.973 13.172 1.00 19.30
                                                              PROT
            512 CG1 VAL 284
     ATOM
                                37.649 11.794 12.959 1.00 16.94
            513 CG2 VAL 284
                                                              PROT
     ATOM
            514 C VAL 284
                              35.113 11.093 15.715 1.00 14.89
                                                             PROT
     ATOM
            515 O VAL 284
                              34.233 11.781 16.219 1.00 10.93
                                                             PROT
     ATOM
            516 N ASP 285
                              35.046 9.768 15.623 1.00 10.68
                                                            PROT
     ATOM
            517 CA ASP 285
                               33.898 9.022 16.114 1.00 20.76
                                                             PROT
     ATOM
     ATOM 518 CB ASP 285
                               34.079 7.518 15.874 1.00 22.99
                                                             PROT
                               33.985 7.130 14.397 1.00 30.01
            519 CG ASP 285
                                                             PROT
     ATOM
           520 OD1 ASP 285
                               33.185 7.735 13.648 1.00 18.56
                                                             PROT
10
     ATOM
                               34.720 6.202 13.993 1.00 27.74
           521 OD2 ASP 285
                                                             PROT
    ATOM
                              33.734 9.274 17.604 1.00 26.87
            522 C ASP 285
     ATOM
                                                            PROT
                              32.609 9.349 18.103 1.00 39.89
    ATOM
            523 O ASP 285
                                                            PROT
            524 N PHE 286
     ATOM
                              34.861 9.405 18.308 1.00 25.45
                                                            PROT
                               34.862 9.654 19.746 1.00 15.66
            525 CA PHE 286
15
     ATOM
                                                             PROT
                               36.284 9.533 20.305 1.00 7.30
            526 CB PHE 286
     ATOM
                                                            PROT
            527 CG PHE 286
                               36.454 10.104 21.703 1.00 17.92
     ATOM
                                                             PROT
            528 CD1 PHE 286
                               35.848 9.499 22.805 1.00 19.35
     ATOM
                                                             PROT
     ATOM
            529 CD2 PHE 286
                               37.229 11.245 21.920 1.00 19.24
                                                             PROT
20
    ATOM
            530 CE1 PHE 286
                               36.014 10.021 24.087 1.00 9.94
                                                             PROT
    ATOM
           531 CE2 PHE 286
                               37.395 11.769 23.207 1.00 11.33
                                                             PROT
     ATOM 532 CZ PHE 286
                              36.786 11.154 24.283 1.00 2.00
                                                             PROT
     ATOM
           533 C PHE 286
                              34.313 11.043 20.030 1.00 17.67
                                                            PROT
     ATOM
           534 O PHE 286
                              33.367 11.201 20.797 1.00 14.36
                                                            PROT
            535 N ALA 287
25
    ATOM
                              34.905 12.056 19.410 1.00 12.57
                                                             PROT
            536 CA ALA 287
                               34.443 13.426 19.622 1.00 12.49
                                                             PROT
     ATOM
    ATOM
            537 CB ALA 287
                               35.250 14.386 18.759 1.00 23.54
                                                             PROT
            538 C ALA 287
                              32.954 13.559 19.307 1.00 9.21
    ATOM
                                                            PROT
            539 O ALA 287
                              32.209 14.205 20.043 1.00 11.68
    ATOM
                                                             PROT
30
    ATOM
            540 N LYS 288
                              32.540 12.929 18.209 1.00 16.43
                                                             PROT
    ATOM
            541 CA LYS 288
                               31.157 12.944 17.736 1.00 16.10
                                                             PROT
    ATOM
            542 CB LYS 288
                               31.003 11.977 16.569 1.00 13.15
                                                             PROT
            543 CG LYS 288
                               31.117 12.636 15.219 1.00 25.55
                                                             PROT
    ATOM
           544 CD LYS 288
                               30.480 11.779 14.136 1.00 32.95
                                                             PROT
    ATOM
           545 CE LYS 288
                              31.279 10.507 13.900 1.00 34.58
35
    ATOM
                                                             PROT
           546 NZ LYS 288
                              30.755 9.721 12.748 1.00 36.93
     ATOM
                                                             PROT
    ATOM
           547 C LYS 288
                              30.154 12.569 18.813 1.00 18.87
                                                            PROT
           548 O LYS 288
    ATOM
                              29.078 13.171 18.917 1.00 12.83
                                                            PROT
            549 N LYS 289
                              30.525 11.574 19.614 1.00 11.81
    ATOM
                                                            PROT
            550 CA LYS 289
40
    ATOM
                               29.674 11.067 20.681 1.00 15.53
                                                             PROT
            551 CB LYS 289
                               30.070 9.631 21.011 1.00 15.88
    ATOM
                                                             PROT
            552 CG LYS 289
                               29.767 8.645 19.911 1.00 20.93
    ATOM
                                                             PROT
            553 CD LYS 289
                               29.140 7.382 20.471 1.00 28.97
    ATOM
                                                             PROT
                              29.951 6.167 20.071 1.00 25.06
    ATOM
            554 CE LYS 289
                                                             PROT
45
    ATOM
            555 NZ LYS 289
                              30.043 6.060 18.590 1.00 39.19
                                                             PROT
    ATOM
            556 C LYS 289
                              29.660 11.884 21.969 1.00 15.95
                                                            PROT
           557 O LYS 289
                              29.205 11.398 23.001 1.00 28.53
    ATOM
                                                            PROT
           558 N LEU 290
                              30.151 13.116 21.919 1.00 10.13
    ATOM
                                                            PROT
            559 CA LEU 290
                               30.155 13.959 23.104 1.00 7.83
    ATOM
                                                             PROT
50
           560 CB LEU 290
                               31.588 14.300 23.532 1.00 14.46
    ATOM
                                                             PROT
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	ATOM	561 CG LEU 290	32.676 13.228 23.542 1.00 11.22	PROT
	ATOM	562 CD1 LEU 290	34.016 13.900 23.678 1.00 3.02	PROT
	ATOM	563 CD2 LEU 290	32.449 12.257 24.686 1.00 9.39	PROT
	ATOM	564 C LEU 290	29.410 15.259 22.849 1.00 7.59	PROT
5	ATOM	565 O LEU 290	29.942 16.148 22.196 1.00 11.01	PROT
	ATOM	566 N PRO 291	28.169 15.381 23.365 1.00 14.33	PROT
	ATOM	567 CD PRO 291	27.515 14.291 24.109 1.00 18.52	PROT
	ATOM	568 CA PRO 291	27.290 16.556 23.240 1.00 6.61	PROT
	ATOM	569 CB PRO 291	26.296 16.400 24.384 1.00 11.95	PROT
10	ATOM	570 CG PRO 291	26.496 15.004 24.929 1.00 20.22	PROT
	ATOM	571 C PRO 291	28.029 17.885 23.332 1.00 14.74	PROT
	ATOM	572 O PRO 291	27.795 18.792 22.537 1.00 26.09	PROT
	ATOM	573 N MET 292	28.917 18.002 24.315 1.00 24.06	PROT
	ATOM	574 CA MET 292	29.697 19.225 24.494 1.00 25.33	PROT
15	ATOM	575 CB MET 292	30.706 19.046 25.628 1.00 26.65	PROT
	ATOM	576 CG MET 292	30.222 19.581 26.962 1.00 26.97	PROT
	ATOM	577 SD MET 292	31.153 18.943 28.362 1.00 29.01	PROT
	ATOM	578 CE MET 292	30.315 17.438 28.685 1.00 17.91	PROT
	ATOM	579 C MET 292	30.430 19.588 23.204 1.00 23.01	PROT
20	ATOM	580 O MET 292	30.478 20.747 22.813 1.00 31.98	PROT
	ATOM	581 N PHE 293	31.007 18.591 22.547 1.00 23.44	PROT
	ATOM	582 CA PHE 293	31.724 18.819 21.297 1.00 24.83	PROT
	ATOM	583 CB PHE 293	32.389 17.529 20.830 1.00 15.05	PROT
	ATOM	584 CG PHE 293	33.214 17.686 19.594 1.00 13.55	PROT
25	ATOM	585 CD1 PHE 293	34.376 18.446 19.614 1.00 19.86	PROT
	ATOM	586 CD2 PHE 293	32.867 17.024 18.425 1.00 22.99	PROT
	ATOM	587 CE1 PHE 293	35.184 18.540 18.495 1.00 18.15	PROT
	ATOM	588 CE2 PHE 293	33.671 17.108 17.291 1.00 20.83	PROT
	ATOM	589 CZ PHE 293	34.831 17.866 17.328 1.00 22.53	PROT
30	ATOM	590 C PHE 293	30.759 19.291 20.222 1.00 27.26	PROT
	ATOM	591 O PHE 293	30.971 20.319 19.577 1.00 28.69	PROT
	ATOM	592 N CYS 294	29.689 18.528 20.040 1.00 29.92	PROT
	ATOM	593 CA CYS 294	28.700 18.855 19.037 1.00 35.54	PROT
	ATOM	594 CB CYS 294	27.540 17.860 19.106 1.00 19.11	PROT
35	ATOM	595 SG CYS 294	27.843 16.358 18.132 1.00 35.66	PROT
	ATOM	596 C CYS 294	28.203 20.291 19.171 1.00 38.84	PROT
	ATOM	597 O CYS 294	28.072 20.995 18.169 1.00 45.94	PROT
	ATOM	598 N GLU 295	27.959 20.739 20.401 1.00 27.34	PROT
	ATOM	599 CA GLU 295	27.472 22.097 20.632 1.00 21.06	PROT
40	ATOM	600 CB GLU 295	27.178 22.306 22.121 1.00 29.78	PROT
	ATOM	601 C GLU 295	28.458 23.158 20.128 1.00 23.67	PROT
	ATOM	602 O GLU 295	28.228 24.357 20.272 1.00 29.89	PROT
	ATOM	603 N LEU 296	29.551 22.715 19.522 1.00 21.46	PROT
	ATOM	604 CA LEU 296	30.545 23.642 19.005 1.00 26.35	PROT
45	ATOM	605 CB LEU 296	31.947 23.128 19.330 1.00 25.17	PROT
	ATOM	606 CG LEU 296	32.419 23.157 20.778 1.00 13.78	PROT
	ATOM	607 CD1 LEU 296	33.593 22.217 20.931 1.00 23.61	PROT
	ATOM	608 CD2 LEU 296	32.814 24.564 21.160 1.00 13.82	PROT
	ATOM	609 C LEU 296	30.415 23.783 17.493 1.00 31.88	PROT
50	ATOM	610 O LEU 296	29.890 22.890 16.827 1.00 45.99	PROT

	ATOM	611 N PRO 297	30.884 24.912 16.932 1.00 27.00	PROT
	ATOM	612 CD PRO 297	31.423 26.037 17.708 1.00 36.12	PROT
	ATOM	613 CA PRO 297	30.856 25.222 15.492 1.00 22.30	PROT
	ATOM	614 CB PRO 297	31.182 26.716 15.424 1.00 16.06	PROT
5	ATOM	615 CG PRO 297	31.107 27.208 16.827 1.00 42.41	PROT
•	ATOM	616 C PRO 297	31.838 24.413 14.642 1.00 28.19	PROT
	ATOM	617 O PRO 297	32.983 24.189 15.036 1.00 39.38	PROT
	ATOM	618 N CYS 298	31.371 24.014 13.457 1.00 35.37	PROT
	ATOM	619 CA CYS 298	32.134 23.233 12.481 1.00 32.41	PROT
10	ATOM	620 CB CYS 298	31.416 23.289 11.112 1.00 40.85	PROT
••	ATOM	621 SG CYS 298	32.431 23.615 9.614 1.00 61.24	PROT
	ATOM	622 C CYS 298	33.596 23.654 12.352 1.00 31.68	PROT
	ATOM	623 O CYS 298	34.474 22.804 12.225 1.00 28.49	PROT
	ATOM	624 N GLU 299	33.869 24.954 12.393 1.00 29.93	PROT
15	ATOM	625 CA GLU 299	35.253 25.407 12.278 1.00 36.38	PROT
	ATOM	626 CB GLU 299	35.346 26.931 12.203 1.00 32.78	PROT
	ATOM	627 CG GLU 299	34.467 27.546 11.167 1.00 43.40	PROT
	ATOM	628 CD GLU 299	33.038 27.593 11.625 1.00 58.19	PROT
	ATOM	629 OE1 GLU 299		PROT
20	ATOM	630 OE2 GLU 299		PROT
	ATOM	631 C GLU 299	36.057 24.932 13.475 1.00 38.89	PROT
	ATOM	632 O GLU 299	37.129 24.342 13.316 1.00 48.67	PROT
	ATOM	633 N ASP 300	35.528 25.186 14.671 1.00 36.49	PROT
	ATOM	634 CA ASP 300	36.201 24.805 15.906 1.00 29.96	PROT
25	ATOM	635 CB ASP 300	35.455 25.391 17.111 1.00 5.33	PROT
	ATOM	636 CG ASP 300	35.830 26.853 17.378 1.00 19.10	PROT
	ATOM	637 OD1 ASP 300	36.491 27.473 16.518 1.00 27.28	PROT
	ATOM	638 OD2 ASP 300	35.470 27.396 18.444 1.00 23.55	PROT
	ATOM	639 C ASP 300	36.380 23.294 16.054 1.00 25.88	PROT
30	ATOM	640 O ASP 300	37.441 22.845 16.484 1.00 19.03	PROT
	ATOM	641 N GLN 301	35.360 22.516 15.689 1.00 6.29	PROT
	ATOM	642 CA GLN 301	35.432 21.055 15.769 1.00 9.51	PROT
	ATOM	643 CB GLN 301	34.170 20.421 15.183 1.00 18.27	PROT
	ATOM	644 CG GLN 301	32.886 20.813 15.875 1.00 28.72	PROT
35	ATOM	645 CD GLN 301	31.676 20.155 15.243 1.00 17.63	PROT
	ATOM	646 OEI GLN 301	31.689 19.823 14.060 1.00 30.65	PROT
	ATOM	647 NE2 GLN 301	30.625 19.965 16.027 1.00 30.44	PROT
	ATOM	648 C GLN 301	36.646 20.491 15.020 1.00 15.48	PROT
	ATOM	649 O GLN 301	37.333 19.584 15.500 1.00 21.96	PROT
40	ATOM	650 N ILE 302	36.891 21.014 13.825 1.00 24.00	PROT
	ATOM	651 CA ILE 302	38.011 20.555 13.026 1.00 28.84	PROT
	ATOM	652 CB ILE 302	37.930 21.112 11.607 1.00 33.13	PROT
	ATOM	653 CG2 ILE 302	39.147 20.690 10.813 1.00 37.90	PROT
	ATOM	654 CG1 ILE 302	36.656 20.610 10.941 1.00 29.63	PROT
45	ATOM	655 CD1 ILE 302	36.296 21.356 9.698 1.00 32.99	PROT
	ATOM	656 C ILE 302	39.308 21.014 13.670 1.00 28.73	PROT
	ATOM	657 O ILE 302	40.219 20.219 13.895 1.00 36.02	PROT
	ATOM	658 N ILE 303	39.396 22.304 13.968 1.00 25.04	PROT
	ATOM	659 CA ILE 303	40.590 22.817 14.603 1.00 24.27	PROT
50	ATOM	660 CB ILE 303	40.414 24.270 15.054 1.00 20.89	PROT

	ATOM		1.686 24.740 15.744 1.00 32.38	PROT
	ATOM	662 CG1 ILE 303 4	0.079 25.158 13.849 1.00 18.88	PROT
	ATOM	663 CD1 ILE 303 4	0.298 26.648 14.079 1.00 5.31	PROT
	ATOM		861 21.948 15.825 1.00 26.92	PROT
5	ATOM	665 O ILE 303 41.	963 21.440 15.997 1.00 31.32	PROT
	ATOM		9.843 21.763 16.659 1.00 11.00	PROT
	ATOM		9.983 20.953 17.854 1.00 7.21	PROT
	ATOM		8.663 20.886 18.613 1.00 2.00	PROT
	ATOM		88.633 21.511 20.012 1.00 8.04	PROT
10	ATOM		39.383 22.812 19.997 1.00 2.00	PROT
	ATOM		37.188 21.729 20.472 1.00 4.99	PROT
	ATOM).441 19.554 17.507 1.00 4.64	PROT
	ATOM		1.368 19.032 18.119 1.00 14.88	PROT
	ATOM		9.807 18.953 16.510 1.00 4.55	PROT
15	ATOM		0.140 17.590 16.093 1.00 7.03	PROT
	ATOM		9.099 17.098 15.104 1.00 3.70	PROT
	ATOM		88.164 16.054 15.691 1.00 10.31	PROT
	ATOM	_	36.744 16.340 15.245 1.00 2.00	PROT
	ATOM		38.629 14.665 15.260 1.00 9.42	PROT
20	ATOM		.527 17.418 15.483 1.00 10.17	PROT
	ATOM		2.174 16.374 15.651 1.00 7.58	PROT
	ATOM		.975 18.442 14.765 1.00 9.98	PROT
	ATOM		3.283 18.408 14.127 1.00 9.14	PROT
	ATOM		3.409 19.558 13.131 1.00 18.85	PROT
25	ATOM		2.815 19.270 11.763 1.00 25.44	PROT
	ATOM		2.198 20.529 11.178 1.00 29.07	PROT
	ATOM		2.698 20.808 9.774 1.00 37.81	PROT
	ATOM		3.867 19.964 9.403 1.00 30.48	PROT
20	ATOM		3.376 18.522 15.175 1.00 7.31	PROT
30	ATOM		5.439 17.919 15.048 1.00 16.95	PROT
	ATOM		4.097 19.295 16.218 1.00 12.67	PROT
	ATOM		15.062 19.484 17.279 1.00 7.25	PROT PROT
	ATOM		5.297 18.269 18.150 1.00 15.08 6.441 17.972 18.488 1.00 20.11	PROT
25	ATOM		6.441 17.972 18.488 1.00 20.11 4.225 17.552 18.481 1.00 8.29	PROT
35	ATOM ATOM		4.286 16.380 19.364 1.00 3.44	PROT
	ATOM		3.097 16.402 20.326 1.00 14.26	PROT
			1.539 15.750 19.634 1.00 21.83	PROT
	ATOM ATOM		1.339 13.730 19.034 1.00 21.83	PROT
40	ATOM		4.502 13.997 19.453 1.00 10.98	PROT
40	ATOM		4.202 14.916 17.420 1.00 10.83	PROT
	ATOM		4.236 13.625 16.752 1.00 3.22	PROT
	ATOM		4.240 13.831 15.240 1.00 15.79	PROT
	ATOM		3.683 12.402 14.319 1.00 25.54	PROT
45	ATOM		5.439 12.767 17.193 1.00 2.00	PROT
73	ATOM		5,251 11.722 17.807 1.00 12.28	PROT
	ATOM		6.663 13.205 16.900 1.00 2.00	PROT
	ATOM		47.858 12.446 17.286 1.00 2.00	PROT
	ATOM		49.122 13.171 16.860 1.00 2.00	PROT
50	ATOM		49.975 12.422 15.880 1.00 5.92	PROT
20	1110141			

	ATOM	711 SD MET 310 50.481 10.805 16.368 1.00 22.47 PROT
	ATOM	712 CE MET 310 52.140 11.112 16.808 1.00 20.84 PROT
	ATOM	713 C MET 310 47.941 12.239 18.793 1.00 11.95 PROT
	ATOM	714 O MET 310 48.455 11.220 19.270 1.00 15.53 PROT
5	ATOM	715 N GLU 311 47.463 13.225 19.542 1.00 6.79 PROT
	ATOM	716 CA GLU 311 47.493 13.139 20.979 1.00 2.00 PROT
	ATOM	717 CB GLU 311 46.932 14.427 21.581 1.00 6.42 PROT
	ATOM	718 CG GLU 311 47.880 15.619 21.436 1.00 8.40 PROT
	ATOM	719 CD GLU 311 47.236 16.940 21.820 1.00 14.10 PROT
10	ATOM	720 OE1 GLU 311 46.157 16.895 22.434 1.00 16.54 PROT
	ATOM	721 OE2 GLU 311 47.795 18.020 21.515 1.00 4.09 PROT
	ATOM	722 C GLU 311 46.683 11.923 21.406 1.00 7.80 PROT
	ATOM	723 O GLU 311 47.195 11.026 22.067 1.00 14.07 PROT
	ATOM	724 N ILE 312 45.425 11.873 21.001 1.00 2.00 PROT
15	ATOM	725 CA ILE 312 44.574 10.752 21.371 1.00 3.60 PROT
	ATOM	726 CB ILE 312 43.114 11.013 20.947 1.00 2.00 PROT
	ATOM	727 CG2 ILE 312 42.277 9.769 21.145 1.00 2.00 PROT
	ATOM	728 CG1 ILE 312 42.579 12.221 21.727 1.00 2.00 PROT
	ATOM	729 CD1 ILE 312 41.118 12.555 21.495 1.00 2.00 PROT
20	ATOM	730 C ILE 312 45.049 9.437 20.760 1.00 8.32 PROT
20	ATOM	731 O ILE 312 44.918 8.373 21.370 1.00 5.58 PROT
	ATOM	732 N MET 313 45.615 9.501 19.563 1.00 3.98 PROT
	ATOM	733 CA MET 313 46.054 8.282 18.905 1.00 8.91 PROT
	ATOM	734 CB MET 313 46.455 8.572 17.462 1.00 25.71 PROT
25	ATOM	735 CG MET 313 45.430 8.111 16.431 1.00 22.86 PROT
23	ATOM	736 SD MET 313 45.955 8.430 14.736 1.00 20.60 PROT
	ATOM	737 CE MET 313 45.412 10.055 14.534 1.00 14.95 PROT
	ATOM	738 C MET 313 47.211 7.634 19.635 1.00 12.95 PROT
	ATOM	739 O MET 313 47.213 6.426 19.857 1.00 22.09 PROT
30	ATOM	740 N SER 314 48.190 8.442 20.021 1.00 10.79 PROT
50	ATOM	741 CA SER 314 49.354 7.935 20.719 1.00 2.00 PROT
	ATOM	742 CB SER 314 50.399 9.042 20.816 1.00 7.24 PROT
	ATOM	743 OG SER 314 50.453 9.815 19.619 1.00 10.89 PROT
	ATOM	744 C SER 314 48.991 7.399 22.105 1.00 8.64 PROT
35	ATOM	745 O SER 314 49.559 6.392 22.558 1.00 5.72 PROT
55	ATOM	746 N LEU 315 48.050 8.062 22.782 1.00 2.00 PROT
	ATOM	747 CA LEU 315 47.628 7.605 24.104 1.00 2.00 PROT
	ATOM	748 CB LEU 315 46.521 8.502 24.671 1.00 2.95 PROT
	ATOM	749 CG LEU 315 45.831 8.096 25.992 1.00 2.00 PROT
40	ATOM	750 CD1 LEU 315 46.876 7.845 27.072 1.00 2.54 PROT
. •	ATOM	751 CD2 LEU 315 44.865 9.182 26.444 1.00 2.00 PROT
	ATOM	752 C LEU 315 47.107 6.182 23.945 1.00 3.25 PROT
	ATOM	753 O LEU 315 47.568 5.253 24.603 1.00 2.00 PROT
	ATOM	754 N ARG 316 46.157 6.010 23.039 1.00 7.28 PROT
45	ATOM	755 CA ARG 316 45.588 4.691 22.808 1.00 13.31 PROT
	ATOM	756 CB ARG 316 44.551 4.758 21.693 1.00 11.11 PROT
	ATOM	757 CG ARG 316 43.545 5.872 21.887 1.00 10.55 PROT
	ATOM	758 CD ARG 316 42.354 5.639 21.012 1.00 10.09 PROT
	ATOM	759 NE ARG 316 41.131 6.149 21.605 1.00 12.29 PROT
50	ATOM	760 CZ ARG 316 39.955 6.127 20.994 1.00 6.99 PROT
	_	

	ATOM	761 NH1 ARG 316	38.880 6.608 21.595 1.00 19.32	PROT
	ATOM	762 NH2 ARG 316	39.853 5.619 19.778 1.00 17.16	PROT
	ATOM	763 C ARG 316	46.666 3.686 22.458 1.00 10.10	PROT
	ATOM	764 O ARG 316	46.549 2.508 22.753 1.00 14.94	PROT
5	ATOM	765 N ALA 317	47.723 4.148 21.819 1.00 6.51	PROT
	ATOM	766 CA ALA 317	48.801 3.243 21.474 1.00 11.04	PROT
	ATOM	767 CB ALA 317	49.749 3.902 20.487 1.00 16.13	PROT
	ATOM	768 C ALA 317	49.539 2.910 22.753 1.00 12.70	PROT
	ATOM	769 O ALA 317	49.822 1.755 23.033 1.00 23.09	PROT
10	ATOM	770 N ALA 318	49.832 3.943 23.534 1.00 14.79	PROT
	ATOM	771 CA ALA 318	50.567 3.779 24.776 1.00 8.38	PROT
	ATOM	772 CB ALA 318	50.727 5.122 25.448 1.00 11.75	PROT
	ATOM	773 C ALA 318	49.941 2.786 25.741 1.00 10.30	PROT
	ATOM	774 O ALA 318	50.585 1.824 26.165 1.00 8.48	PROT
15	ATOM	775 N VAL 319	48.680 3.011 26.083 1.00 7.87	PROT
••	ATOM	776 CA VAL 319	48.002 2.131 27.027 1.00 9.64	PROT
	ATOM	777 CB VAL 319	46.579 2.622 27.334 1.00 2.57	PROT
	ATOM	778 CG1 VAL 319	46.644 3.929 28.127 1.00 5.09	PROT
	ATOM	779 CG2 VAL 319	45.807 2.823 26.043 1.00 5.15	PROT
20	ATOM	780 C VAL 319	47.930 0.695 26.541 1.00 11.68	PROT
	ATOM	781 O VAL 319	47.440 -0.171 27.254 1.00 16.32	PROT
	ATOM	782 N ARG 320	48,415 0.444 25.329 1.00 16.40	PROT
	ATOM	783 CA ARG 320	48,405 -0.902 24.767 1.00 13.20	PROT
	ATOM	784 CB ARG 320	47.736 -0.918 23.393 1.00 2.00	PROT
25	ATOM	785 CG ARG 320	46.310 -0.405 23.420 1.00 14.07	PROT
	ATOM	786 CD ARG 320	45.283 -1.460 23.035 1.00 19.69	PROT
	ATOM	787 NE ARG 320	44.168 -0.868 22.292 1.00 36.52	PROT
	ATOM	788 CZ ARG 320	42.912 -1.313 22.322 1.00 47.43	PROT
	ATOM	789 NH1 ARG 320	41.966 -0.705 21.609 1.00 43.57	PROT
30	ATOM	790 NH2 ARG 320	42.596 -2.367 23.061 1.00 49.93	PROT
	ATOM	791 C ARG 320	49.835 -1.391 24.662 1.00 15.45	PROT
	ATOM	792 O ARG 320	50.167 -2.218 23.809 1.00 24.78	PROT
	ATOM	793 N TYR 321	50.684 -0.860 25.537 1.00 13.68	PROT
	ATOM	794 CA TYR 321	52.085 -1.258 25.572 1.00 18.80	PROT
35	ATOM	795 CB TYR 321	52.925 -0.208 26.295 1.00 9.64	PROT
	ATOM	796 CG TYR 321	54.313 -0.685 26.622 1.00 11.20	PROT
	ATOM	797 CD1 TYR 321	55.211 -1.005 25.612 1.00 2.00	PROT
	ATOM	798 CE1 TYR 321	56.483 -1.461 25.906 1.00 9.63	PROT
	ATOM	799 CD2 TYR 321	54.727 -0.834 27.943 1.00 18.93	PROT
40	ATOM	800 CE2 TYR 321	56.003 -1.293 28.250 1.00 19.49	PROT
	ATOM	801 CZ TYR 321	56.874 -1.604 27.225 1.00 14.75	PROT
	ATOM	802 OH TYR 321	58.137 -2.053 27.518 1.00 22.96	PROT
	ATOM	803 C TYR 321	52.209 -2.607 26.287 1.00 19.74	PROT
	ATOM	804 O TYR 321	51.483 -2.889 27.242 1.00 31.56	PROT
45	ATOM	805 N ASP 322	53.136 -3.435 25.823 1.00 26.35	PROT
	ATOM	806 CA ASP 322	53.346 -4.759 26.392 1.00 22.38	PROT
	ATOM	807 CB ASP 322	52.982 -5.814 25.353 1.00 33.63	PROT
	ATOM	808 CG ASP 322	52.601 -7.128 25.970 1.00 40.70	PROT
	ATOM	809 OD1 ASP 322	51.539 -7.658 25.591 1.00 48.18	PROT
50	ATOM	810 OD2 ASP 322	53.358 -7.628 26.826 1.00 38.91	PROT

	ATOM	811 C ASP 322	54.800 -4.928 26.776 1.00 23.51	PROT
	ATOM	812 O ASP 322	55.683 -4.844 25.924 1.00 37.80	PROT
	ATOM	813 N PRO 323	55.076 -5.160 28.066 1.00 24.06	PROT
	ATOM	814 CD PRO 323	54.130 -5.258 29.187 1.00 19.35	PROT
5	ATOM	815 CA PRO 323	56.462 -5.339 28.507 1.00 23.60	PROT
	ATOM	816 CB PRO 323	56.390 -5.121 30.007 1.00 3.90	PROT
	ATOM	817 CG PRO 323	55.031 -5.570 30.360 1.00 14.06	PROT
	ATOM	818 C PRO 323	56.949 -6.736 28.151 1.00 21.79	PROT
	ATOM	819 O PRO 323	58.149 -7.003 28.119 1.00 27.28	PROT
10	ATOM	820 N GLU 324	56.009 -7.633 27.889 1.00 37.63	PROT
	ATOM	821 CA GLU 324	56.366 -8.993 27.524 1.00 42.63	PROT
	ATOM	822 CB GLU 324	55.133 -9.885 27.551 1.00 37.58	PROT
	ATOM	823 C GLU 324	56.971 -8.956 26.124 1.00 43.28	PROT
	ATOM	824 O GLU 324	58.154 -9.239 25.938 1.00 43.14	PROT
15	ATOM	825 N SER 325	56.153 -8.586 25.142 1.00 31.72	PROT
	ATOM	826 CA SER 325	56.607 -8.508 23.765 1.00 30.34	PROT
	ATOM	827 CB SER 325	55.413 -8.522 22.814 1.00 17.63	PROT
	ATOM	828 OG SER 325	54.356 -7.729 23.315 1.00 31.90	PROT
	ATOM	829 C SER 325	57.441 -7.257 23.519 1.00 31.94	PROT
20	ATOM	830 O SER 325	58.146 -7.169 22.513 1.00 45.47	PROT
	ATOM	831 N GLU 326	57.359 -6.289 24.429 1.00 31.10	PROT
	ATOM	832 CA GLU 326	58.119 -5.050 24.281 1.00 31.43	PROT
	ATOM	833 CB GLU 326	59.598 -5.382 24.091 1.00 30.39	PROT
	ATOM	834 CG GLU 326	60.552 -4.342 24.612 1.00 35.00	PROT
25	ATOM	835 CD GLU 326	61.738 -4.965 25.304 1.00 29.12	PROT
	ATOM	836 OE1 GLU 326	61.525 -5.579 26.370 1.00 39.21	PROT
	ATOM	837 OE2 GLU 326	62.872 -4.844 24.788 1.00 29.11	PROT
	ATOM	838 C GLU 326	57.605 -4.283 23.063 1.00 28.37	PROT
	ATOM	839 O GLU 326	58.382 -3.677 22.321 1.00 26.51	PROT
30	ATOM	840 N THR 327	56.290 -4.301 22.873 1.00 23.71	PROT
	ATOM	841 CA THR 327	55.674 -3.648 21.720 1.00 22.11	PROT
	ATOM	842 CB THR 327	55.298 -4.705 20.652 1.00 28.08	PROT
	ATOM	843 OG1 THR 327	54.226 -5.524 21.145 1.00 16.87	PROT
	ATOM	844 CG2 THR 327	56.494 -5.597 20.340 1.00 24.03	PROT
35	ATOM	845 C THR 327	54.420 -2.824 22.046 1.00 22.42	PROT
	ATOM	846 O THR 327	53.928 -2.830 23.172 1.00 17.50	PROT
	ATOM	847 N LEU 328	53.914 -2.122 21.038 1.00 17.28	PROT
	ATOM	848 CA LEU 328	52.728 -1.285 21.171 1.00 14.83	PROT
	ATOM	849 CB LEU 328	53.065 0.157 20.806 1.00 15.27	PROT
40	ATOM	850 CG LEU 328	53.693 1.036 21.879 1.00 10.50	PROT
	ATOM	851 CD1 LEU 328	54.137 2.336 21.254 1.00 16.75	PROT
	ATOM	852 CD2 LEU 328	52.682 1.285 22.979 1.00 20.19	PROT
	ATOM	853 C LEU 328	51.687 -1.804 20.198 1.00 18.16	PROT
	ATOM	854 O LEU 328	52.035 -2.508 19.254 1.00 23.88	PROT
45	ATOM	855 N THR 329	50.421 -1.450 20.402 1.00 9.40	PROT
	ATOM	856 CA THR 329	49.389 -1.920 19.495 1.00 8.26	PROT
	ATOM	857 CB THR 329	48.460 -2.888 20.199 1.00 8.67	PROT
	ATOM	858 OG1 THR 329	49.213 -4.052 20.577 1.00 13.23	PROT
	ATOM	859 CG2 THR 329	47.308 -3.289 19.270 1.00 2.00	PROT
50	ATOM	860 C THR 329	48.569 -0.841 18.800 1.00 16.65	PROT

	ATOM	861 O THR 329	47.726 -0.158 19.406 1.00 17.20	PROT
	ATOM	862 N LEU 330	48.808 -0.725 17.495 1.00 21.56	PROT
	ATOM	863 CA LEU 330	48.138 0.258 16.655 1.00 20.95	PROT
	ATOM	864 CB LEU 330	49.106 0.676 15.539 1.00 17.36	PROT
5	ATOM	865 CG LEU 330	50.570 0.797 16.028 1.00 12.86	PROT
	ATOM	866 CD1 LEU 330	51.531 0.521 14.898 1.00 10.10	PROT
	ATOM	867 CD2 LEU 330	50.830 2.180 16.600 1.00 2.00	PROT
	ATOM	868 C LEU 330	46.803 -0.258 16.097 1.00 21.35	PROT
	ATOM	869 O LEU 330	46.655 -1.444 15.791 1.00 21.93	PROT
10	ATOM	870 N ASN 331	45.834 0.648 15.987 1.00 27.76	PROT
	ATOM	871 CA ASN 331	44.487 0.338 15.498 1.00 28.09	PROT
	ATOM	872 CB ASN 331	44.460 0.275 13.971 1.00 24.95	PROT
	ATOM	873 CG ASN 331	43.074 0.540 13.397 1.00 33.45	PROT
	ATOM	874 OD1 ASN 331	42.512 -0.305 12.701 1.00 38.21	PROT
15	ATOM	875 ND2 ASN 331	42.522 1.715 13.680 1.00 24.73	PROT
	ATOM	876 C ASN 331	43.946 -0.967 16.075 1.00 32.03	PROT
	ATOM	877 O ASN 331	43.166 -1.668 15.431 1.00 35.49	PROT
	ATOM	878 N GLY 332	44.357 -1.282 17.299 1.00 40.24	PROT
	ATOM	879 CA GLY 332	43.894 -2.495 17.941 1.00 38.04	PROT
20	ATOM	880 C GLY 332	44.009 -3.665 16.998 1.00 40.09	PROT
	ATOM	881 O GLY 332	43.001 -4.225 16.563 1.00 45.79	PROT
	ATOM	882 N GLU 333	45.249 -4.013 16.664 1.00 41.60	PROT
	ATOM	883 CA GLU 333	45.539 -5.126 15.763 1.00 36.28	PROT
	ATOM	884 CB GLU 333	44.752 -4.978 14.454 1.00 46.39	PROT
25	ATOM	885 CG GLU 333	44.745 -3.580 13.862 1.00 58.03	PROT
	ATOM	886 CD GLU 333	43.883 -3.485 12.610 1.00 67.00	PROT
	ATOM	887 OE1 GLU 333	44.446 -3.282 11.511 1.00 67.51	PROT
	ATOM	888 OE2 GLU 333	42.644 -3.615 12.727 1.00 71.01	PROT
	ATOM	889 C GLU 333	47.027 -5.266 15.446 1.00 33.13	PROT
30	ATOM	890 O GLU 333	47.563 -6.366 15.486 1.00 27.97	PROT
	ATOM	891 N MET 334	47.692 -4.152 15.143 1.00 27.00	PROT
	ATOM	892 CA MET 334	49.111 -4.188 14.798 1.00 29.83	PROT
	ATOM	893 CB MET 334	49.416 -3.159 13.699 1.00 26.04	PROT
	ATOM	894 CG MET 334	50.561 -3.588 12.765 1.00 28.06	PROT
35	ATOM	895 SD MET 334	51.263 -2.273 11.736 1.00 28.46	PROT
	ATOM	896 CE MET 334	50.021 -2.123 10.497 1.00 22.48	PROT
	ATOM	897 C MET 334	50.087 -3.995 15.959 1.00 33.52	PROT
	ATOM	898 O MET 334	50.071 -2.962 16.631 1.00 35.81	PROT
	ATOM	899 N ALA 335	50.942 -4.996 16.171 1.00 27.46	PROT
40	ATOM	900 CA ALA 335	51.948 -4.976 17.234 1.00 29.69	PROT
	ATOM	901 CB ALA 335	51.966 -6.314 17.965 1.00 12.67	PROT
	ATOM	902 C ALA 335	53.336 -4.682 16.662 1.00 31.74	PROT
	ATOM	903 O ALA 335	53.943 -5.530 16.009 1.00 43.66	PROT
	ATOM	904 N VAL 336	53.848 -3.489 16.923 1.00 23.98	PROT
45	ATOM	905 CA VAL 336	55.151 -3.118 16.405 1.00 21.32	PROT
	ATOM	906 CB VAL 336	55.028 -1.873 15.504 1.00 17.37	PROT
	ATOM	907 CG1 VAL 336	53.945 -2.104 14.462 1.00 14.88	PROT
	ATOM	908 CG2 VAL 336	54.686 -0.648 16.339 1.00 15.53	PROT
	ATOM	909 C VAL 336	56.150 -2.852 17.526 1.00 22.72	PROT
50	ATOM	910 O VAL 336	55.763 -2.540 18.651 1.00 25.15	PROT
	111 0111	7.0 C TIL 550	JJ., JJ -2.J 10 10.UJ1 1.UU 2J.1J	

	ATOM	911 N THR 337	57.435 -3.001 17.220 1.00 19.21	PROT
	ATOM	912 CA THR 337	58.476 -2.765 18.205 1.00 20.31	PROT
	ATOM	913 CB THR 337	59.752 -3.578 17.884 1.00 14.76	PROT
	ATOM	914 OG1 THR 337	59.957 -3.616 16.467 1.00 16.43	PROT
5	ATOM	915 CG2 THR 337	59.615 -4.995 18.393 1.00 7.08	PROT
	ATOM	916 C THR 337	58.785 -1.272 18.157 1.00 24.20	PROT
	ATOM	917 O THR 337	58.322 -0.591 17.245 1.00 28.05	PROT
	ATOM	918 N ARG 338	59.548 -0.766 19.134 1.00 27.55	PROT
	ATOM	919 CA ARG 338	59.917 0.655 19.197 1.00 16.80	PROT
10	ATOM	920 CB ARG 338	60.757 0.942 20.446 1.00 17.04	PROT
	ATOM	921 CG ARG 338	61.687 2.149 20.303 1.00 9.79	PROT
	ATOM	922 CD ARG 338	62.666 2.276 21.458 1.00 2.00	PROT
	ATOM	923 NE ARG 338	61.994 2.128 22.739 1.00 20.70	PROT
	ATOM	924 CZ ARG 338	61.897 3.083 23.657 1.00 12.04	PROT
15	ATOM	925 NH1 ARG 338	61.261 2.840 24.784 1.00 27.11	PROT
	ATOM	926 NH2 ARG 338	62.436 4.272 23.459 1.00 22.23	PROT
	ATOM	927 C ARG 338	60.702 1.085 17.968 1.00 21.26	PROT
	ATOM	928 O ARG 338	60.338 2.049 17.295 1.00 16.40	PROT
	ATOM	929 N GLY 339	61.792 0.374 17.693 1.00 31.57	PROT
20	ATOM	930 CA GLY 339	62.609 0.696 16.540 1.00 32.42	PROT
	ATOM	931 C GLY 339	61.816 0.534 15.254 1.00 30.08	PROT
	ATOM	932 O GLY 339	61.932 1.342 14.328 1.00 25.82	PROT
	ATOM	933 N GLN 340	61.008 -0.520 15.192 1.00 16.60	PROT
	ATOM	934 CA GLN 340	60.191 -0.768 14.012 1.00 14.08	PROT
25	ATOM	935 CB GLN 340	59.199 -1.884 14.301 1.00 5.73	PROT
	ATOM	936 CG GLN 340	58.849 -2.697 13.100 1.00 16.15	PROT
	ATOM	937 CD GLN 340	58.577 -4.141 13.442 1.00 22.46	PROT
	ATOM	938 OE1 GLN 340	57.767 -4.450 14.316 1.00 30.45	PROT
	ATOM	939 NE2 GLN 340	59.254 -5.040 12.749 1.00 34.19	PROT
30	ATOM	940 C GLN 340	59.452 0.521 13.632 1.00 22.07	PROT
	ATOM	941 O GLN 340	59.707 1.103 12.576 1.00 21.13	PROT
	ATOM	942 N LEU 341	58.561 0.976 14.518 1.00 27.88	PROT
	ATOM	943 CA LEU 341	57.778 2.197 14.306 1.00 21.82	PROT
	ATOM	944 CB LEU 341	56.813 2.418 15.483 1.00 10.20	PROT
35	ATOM	945 CG LEU 341	55.930 3.682 15.534 1.00 16.27	PROT
	ATOM	946 CD1 LEU 341	54.777 3.618 14.518 1.00 13.27	PROT
	ATOM	947 CD2 LEU 341	55.370 3.822 16.935 1.00 10.68	PROT
	ATOM	948 C LEU 341	58.683 3.413 14.138 1.00 13.98	PROT
	ATOM	949 O LEU 341	58.315 4.386 13.486 1.00 7.94	PROT
40	ATOM	950 N LYS 342	59.867 3.361 14.734 1.00 11.48	PROT
	ATOM	951 CA LYS 342	60.804 4.465 14.613 1.00 17.77	PROT
	ATOM	952 CB LYS 342	62.063 4.213 15.459 1.00 13.58	PROT
	ATOM	953 CG LYS 342	63.219 5.173 15.140 1.00 13.27	PROT
	ATOM	954 CD LYS 342	64.173 5.358 16.319 1.00 5.44	PROT
45	ATOM	955 CE LYS 342	64.500 6.829 16.546 1.00 5.47	PROT
-	ATOM	956 NZ LYS 342	65.721 7.019 17.388 1.00 4.98	PROT
	ATOM	957 C LYS 342	61.184 4.579 13.141 1.00 19.97	PROT
	ATOM	958 O LYS 342	60.939 5.595 12.501 1.00 20.34	PROT
	ATOM	959 N ASN 343	61.764 3.510 12.605 1.00 26.88	PROT
50	ATOM	960 CA ASN 343	62.196 3.470 11.219 1.00 22.34	PROT

ATOM 962 CG ASN 343 64.060 1.894 11.758 1.00 18.77 PROT ATOM 964 ND2 ASN 343 64.755 2.848 12.117 1.00 14.12 PROT PROT ATOM 964 ND2 ASN 343 64.340 0.634 12.083 1.00 12.72 PROT ATOM 966 CA ASN 343 61.091 3.736 10.224 1.00 20.40 PROT ATOM 967 N GLY 344 59.908 3.200 10.494 1.00 12.62 PROT ATOM 968 CA GLY 344 58.229 4.796 9.451 1.00 14.56 PROT ATOM 970 O GLY 344 58.229 4.796 9.451 1.00 14.56 PROT ATOM 971 N GLY 345 58.902 5.795 10.030 1.00 16.51 ATOM 972 CA GLY 345 58.248 8.112 11.046 1.00 25.64 PROT ATOM 973 C GLY 345 58.248 9.331 10.849 1.00 23.32 PROT ATOM 974 O GLY 345 58.249 9.331 10.849 1.00 23.32 PROT ATOM 975 N LEU 346 58.099 7.588 12.260 1.00 22.22 PROT ATOM 976 CA LEU 346 57.070 7.700 14.474 1.00 3.92 PROT ATOM 978 CG LEU 346 57.070 7.700 14.474 1.00 3.92 PROT ATOM 978 CG LEU 346 55.566 7.538 14.193 1.00 5.92 PROT ATOM 980 CD2 LEU 346 59.102 10.153 14.554 1.00 17.36 PROT ATOM 981 C LEU 346 59.102 10.153 14.554 1.00 17.36 PROT ATOM 982 O LEU 346 59.102 10.153 14.554 1.00 17.36 PROT ATOM 988 CA VAL 348 ATOM 987 CG LEU 346 59.102 10.153 14.554 1.00 17.36 PROT ATOM 988 CA VAL 348 62.942 11.802 19.836 1.00 2.00 PROT ATOM 987 O GLY 347 60.266 8.312 14.001 1.00 12.09 PROT ATOM 988 CA VAL 348 62.946 11.6.790 1.00 6.31 PROT ATOM 989 CB VAL 348 62.942 11.802 19.836 1.00 2.00 PROT ATOM 990 CGI VAL 348 ATOM 990 CGI VAL 349 ATOM 990 CGI VA		ATOM	961 CB ASN 343	62.829 2.123 10.929 1.00 4.80 64.060 1.894 11.758 1.00 18.77	PROT PROT
ATOM 964 ND2 ASN 343 64.340 0.634 12.083 1.00 12.72 PROT ATOM 965 C ASN 343 61.091 3.736 10.224 1.00 20.40 PROT ATOM 966 C ASN 343 61.099 4.417 9.232 1.00 20.76 PROT ATOM 967 N GLY 344 59.908 3.200 10.494 1.00 12.62 PROT ATOM 968 CA GLY 344 58.775 3.382 9.603 1.00 6.27 PROT ATOM 970 C GLY 344 58.775 3.382 9.603 1.00 6.27 PROT ATOM 971 N GLY 345 58.902 5.795 10.030 1.00 16.51 PROT ATOM 972 CA GLY 345 58.902 5.795 10.030 1.00 16.51 PROT ATOM 973 C GLY 345 58.248 9.7166 9.869 1.00 20.04 PROT ATOM 974 O GLY 345 58.248 9.331 10.849 1.00 22.32 PROT ATOM 975 N LEU 346 58.099 7.588 12.260 1.00 22.32 PROT ATOM 976 CA LEU 346 57.070 7.700 14.474 1.00 3.92 PROT ATOM 978 CG LEU 346 59.102 10.153 14.594 1.00 14.94 PROT ATOM 980 CD2 LEU 346 59.102 10.153 14.594 1.00 17.36 PROT ATOM 983 N GLY 347 61.458 48.885 13.973 1.00 2.00 PROT ATOM 984 CA GLY 347 61.459 8.963 16.090 1.00 6.31 PROT ATOM 986 O GLY 347 61.459 8.963 16.090 1.00 13.15 PROT ATOM 987 N VAL 348 62.751 11.646 18.342 1.00 10.374 PROT ATOM 989 CB VAL 348 62.751 11.646 18.342 1.00 9.26 PROT ATOM 990 CGI VAL 348 60.763 10.216 18.650 1.00 6.61 PROT ATOM 991 CG2 VAL 348 60.763 10.321 18.306 1.00 2.00 PROT ATOM 992 C VAL 348 60.763 10.321 18.306 1.00 2.00 PROT ATOM 994 N VAL 349 57.421 10.825 18.00 1.00 6.11 PROT ATOM 995 CA VAL 349 58.386 10.034 18.306 1.00 2.00 PROT ATOM 996 CB VAL 349 57.421 10.826 1.00 3.12 PROT ATOM 996 CB VAL 349 57.421 10.826 1.00 3.12 PROT ATOM 997 CGI VAL 349 58.386 10.342 18.306 1.00 2.00 PROT ATOM 998 CG2 VAL 349 57.284 8.726 19.664 1.00 15.02 PROT ATOM 990 CGI VAL 349 57.284 8.726 19.664 1.00 15.02 PROT ATOM 1000 N VAL 349 57.284 8.726 19.664 1.00 15.02 PROT ATOM 1000 N SER 350 58.695 5.561 17.382 1.00 9.48 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.48 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.58 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.58 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.58 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.58 PROT ATOM 1000 C SER 350 58.695 5.561 17.382 1.00 9.58 PROT ATOM				_	
5 ATOM 965 C ASN 343 61.091 3.736 10.224 1.00 20.76 PROT ATOM 966 O ASN 343 61.309 4.417 9.232 1.00 20.76 PROT ATOM 968 CA GLY 344 58.775 3.382 9.603 1.00 6.27 PROT ATOM 969 C GLY 344 58.229 4.796 9.451 1.00 14.56 PROT ATOM 971 N GLY 345 58.283 9.795 10.03 1.00 16.51 PROT ATOM 972 CA GLY 345 58.248 8.112 11.046 1.00 25.64 PROT ATOM 974 O GLY 345 58.248 8.112 11.046 1.00 25.64 PROT ATOM 976 C B LEU 346 58.094 7.588 12.260 1.00 22.22 PROT ATOM 976 C B LEU <td></td> <td></td> <td></td> <td></td> <td></td>					
ATOM 966 O ASN 433	5				
ATOM 967 N GLY 344 ATOM 968 CA GLY 344 ATOM 968 CA GLY 344 ATOM 970 O GLY 344 ATOM 970 O GLY 344 ATOM 971 N GLY 345 ATOM 971 N GLY 345 ATOM 972 CA GLY 345 ATOM 973 C GLY 345 ATOM 974 O GLY 345 ATOM 975 N LEU 346 ATOM 975 N LEU 346 ATOM 976 CA LEU 346 ATOM 977 CB LEU 346 ATOM 977 CB LEU 346 ATOM 978 CG LEU 346 ATOM 981 C LEU 346 ATOM 981 C LEU 346 ATOM 982 O LEU 346 ATOM 984 CA GLY 347 ATOM 984 CA GLY 347 ATOM 985 C GLY 347 ATOM 985 C GLY 347 ATOM 986 O GLY 347 ATOM 987 N VAL 348 ATOM 980 CD2 VAL 348 ATOM 990 CGI VAL 348 ATOM 991 CG2 VAL 348 ATOM 994 N VAL 349 ATOM 995 CA VAL 349 ATOM 996 CB VAL 349 ATOM 997 CGI VAL 349 ATOM 1000 C VAL 349 ATOM 1000 C VAL 349 ATOM 1000 C SER 350 ATOM 1000 C	3				
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40 ATOM 1000 O VAL 349 57.284 8.726 19.664 1.00 15.02 PROT ATOM 1001 N SER 350 58.446 7.943 17.933 1.00 7.42 PROT ATOM 1002 CA SER 350 58.087 6.590 18.315 1.00 12.87 PROT ATOM 1003 CB SER 350 58.695 5.561 17.382 1.00 9.48 PROT ATOM 1004 OG SER 350 58.529 4.269 17.931 1.00 10.82 PROT ATOM 1005 C SER 350 58.628 6.364 19.717 1.00 15.55 PROT ATOM 1006 O SER 350 57.963 5.761 20.558 1.00 25.88 PROT ATOM 1007 N ASP 351 59.838 6.863 19.950 1.00 16.38 PROT ATOM 1009 CB ASP <td< td=""><td></td><td></td><td></td><td></td><td></td></td<>					
ATOM 1001 N SER 350 58.446 7.943 17.933 1.00 7.42 PROT ATOM 1002 CA SER 350 58.087 6.590 18.315 1.00 12.87 PROT ATOM 1003 CB SER 350 58.695 5.561 17.382 1.00 9.48 PROT ATOM 1004 OG SER 350 58.529 4.269 17.931 1.00 10.82 PROT ATOM 1005 C SER 350 58.628 6.364 19.717 1.00 15.55 PROT ATOM 1006 O SER 350 57.963 5.761 20.558 1.00 25.88 PROT ATOM 1007 N ASP 351 59.838 6.863 19.950 1.00 16.38 PROT ATOM 1008 CA ASP 351 60.522 6.743 21.230 1.00 9.58 PROT ATOM 1009 CB ASP 351 61.861 7.469 21.176 1.00 7.32 PROT	40				
ATOM 1002 CA SER 350 58.087 6.590 18.315 1.00 12.87 PROT ATOM 1003 CB SER 350 58.695 5.561 17.382 1.00 9.48 PROT ATOM 1004 OG SER 350 58.529 4.269 17.931 1.00 10.82 PROT ATOM 1005 C SER 350 58.628 6.364 19.717 1.00 15.55 PROT ATOM 1006 O SER 350 57.963 5.761 20.558 1.00 25.88 PROT ATOM 1007 N ASP 351 59.838 6.863 19.950 1.00 16.38 PROT ATOM 1008 CA ASP 351 60.522 6.743 21.230 1.00 9.58 PROT ATOM 1009 CB ASP 351 61.861 7.469 21.176 1.00 7.32 PROT	. •				
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45 ATOM 1005 C SER 350 58.628 6.364 19.717 1.00 15.55 PROT ATOM 1006 O SER 350 57.963 5.761 20.558 1.00 25.88 PROT ATOM 1007 N ASP 351 59.838 6.863 19.950 1.00 16.38 PROT ATOM 1008 CA ASP 351 60.522 6.743 21.230 1.00 9.58 PROT ATOM 1009 CB ASP 351 61.861 7.469 21.176 1.00 7.32 PROT					
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ATOM 1009 CB ASP 351 61.861 7.469 21.176 1.00 7.32 PROT		ATOM			
		ATOM	1008 CA ASP 351		PROT
50 ATOM 1010 CG ASP 351 62.989 6.576 20.742 1.00 24.16 PROT					
	50	ATOM	1010 CG ASP 351	62.989 6.576 20.742 1.00 24.16	PROT

	ATOM	1011 OD1 ASP 351	64.011 7.110 20.275 1.00 30.24	PROT
	ATOM	1012 OD2 ASP 351	62.866 5.343 20.869 1.00 33.85	PROT
	ATOM		59.695 7.360 22.334 1.00 17.01	PROT
	ATOM		59.605 6.822 23.435 1.00 26.28	PROT
5	ATOM		59.100 8.508 22.032 1.00 13.51	PROT
	ATOM	1016 CA ALA 352	58.294 9.224 23.004 1.00 5.19	PROT
	ATOM	1017 CB ALA 352	57.914 10.593 22.452 1.00 2.00	PROT
	ATOM		57.055 8.432 23.374 1.00 2.00	PROT
	ATOM		56.701 8.360 24.535 1.00 7.20	PROT
10	ATOM			PROT
	ATOM		55.201 7.049 22.677 1.00 5.90	PROT
	ATOM		54.468 6.626 21.381 1.00 5.87	PROT
	ATOM		53.113 6.049 21.732 1.00 2.00	PROT
	ATOM	1024 CG1 ILE 353	54.349 7.831 20.428 1.00 3.91	PROT
15	ATOM	1025 CD1 ILE 353	53.330 7.664 19.294 1.00 2.00	PROT
	ATOM		5.554 5.795 23.484 1.00 12.46	PROT
	ATOM		4.848 5.426 24.428 1.00 11.74	PROT
	ATOM		56.644 5.131 23.122 1.00 19.57	PROT
	ATOM	1029 CA PHE 354	57.034 3.944 23.862 1.00 14.42	PROT
20	ATOM	1030 CB PHE 354	58.256 3.270 23.209 1.00 3.70	PROT
	ATOM	1031 CG PHE 354	57.890 2.141 22.284 1.00 9.42	PROT
	ATOM	1032 CD1 PHE 354	57.427 2.401 20.995 1.00 12.33	PROT
	ATOM	1033 CD2 PHE 354	57.912 0.822 22.727 1.00 15.63	PROT
25	ATOM	1034 CE1 PHE 354	56.982 1.366 20.165 1.00 6.67 57.468 -0.224 21.900 1.00 16.53	PROT
25	ATOM	1035 CE2 PHE 354 1036 CZ PHE 354		PROT PROT
	ATOM ATOM		57.002 0.053 20.620 1.00 11.61 57.322 4.346 25.307 1.00 18.55	PROT
	ATOM		56.796 3.740 26.233 1.00 16.67	PROT
	ATOM		58.125 5.392 25.491 1.00 12.83	PROT
30	ATOM	1040 CA ASP 355	58.486 5.881 26.818 1.00 5.31	PROT
50	ATOM	1041 CB ASP 355	59.351 7.132 26.697 1.00 9.38	PROT
	ATOM	1042 CG ASP 355	60.805 6.814 26.428 1.00 5.96	PROT
	ATOM	1043 OD1 ASP 355	61.112 5.683 26.016 1.00 8.53	PROT
	ATOM	1044 OD2 ASP 355	61.650 7.706 26.628 1.00 15.51	PROT
35	ATOM		57.252 6.199 27.659 1.00 10.27	PROT
	ATOM		57.231 5.972 28.871 1.00 21.86	PROT
	ATOM		56.224 6.726 27.014 1.00 4.18	PROT
	ATOM	1048 CA LEU 356	54.988 7.061 27.697 1.00 2.07	PROT
	ATOM	1049 CB LEU 356	54.086 7.865 26.771 1.00 2.24	PROT
40	ATOM	1050 CG LEU 356	52.694 8.229 27.266 1.00 3.11	PROT
	ATOM	1051 CD1 LEU 356	52.771 9.317 28.323 1.00 2.00	PROT
	ATOM	1052 CD2 LEU 356	51.877 8.709 26.086 1.00 2.00	PROT
	ATOM	1053 C LEU 356	54.281 5.786 28.091 1.00 9.17	PROT
	ATOM	1054 O LEU 356	53.831 5.644 29.221 1.00 14.77	PROT
45	ATOM	1055 N GLY 357	54.183 4.856 27.147 1.00 13.10	PROT
	ATOM	1056 CA GLY 357	53.515 3.597 27.413 1.00 6.91	PROT
	ATOM		54.113 2.879 28.598 1.00 8.33	PROT
	ATOM		53.400 2.426 29.492 1.00 9.09	PROT
	ATOM		55.435 2.768 28.607 1.00 12.61	PROT
50	ATOM	1060 CA MET 358	56.112 2:091 29.692 1.00 10.53	PROT

	ATOM	1061 CB MET 358	57.626 2.153 29.498 1.00 5.45	PROT
	ATOM	1062 CG MET 358	58.138 1.507 28.210 1.00 15.15	PROT
	ATOM	1063 SD MET 358	59.971 1.352 28.113 1.00 17.63	PROT
	ATOM	1064 CE MET 358	60.445 3.023 27.774 1.00 20.56	PROT
5	ATOM	1065 C MET 358	55.714 2.809 30.972 1.00 15.08	PROT
	ATOM	1066 O MET 358	55.241 2.191 31.920 1.00 27.69	PROT
	ATOM	1067 N SER 359	55.875 4.125 30.984 1.00 20.67	PROT
	ATOM	1068 CA SER 359	55.551 4.924 32.158 1.00 19.72	PROT
	ATOM	1069 CB SER 359	55.831 6.398 31.861 1.00 19.98	PROT
10	ATOM	1070 OG SER 359	54.753 7.220 32.262 1.00 33.66	PROT
	ATOM	1071 C SER 359	54.115 4.757 32.656 1.00 22.67	PROT
	ATOM	1072 O SER 359	53.849 4.837 33.860 1.00 22.94	PROT
	ATOM	1073 N LEU 360	53.197 4.514 31.727 1.00 20.55	PROT
	ATOM	1074 CA LEU 360	51.785 4.360 32.054 1.00 17.01	PROT
15	ATOM	1075 CB LEU 360	50,934 4.578 30.802 1.00 2.60	PROT
	ATOM	1076 CG LEU 360	50.674 5.988 30.291 1.00 6.99	PROT
	ATOM	1077 CD1 LEU 360	49.589 5.935 29.236 1.00 4.15	PROT
	ATOM	1078 CD2 LEU 360	50.247 6.892 31.432 1.00 18.93	PROT
	ATOM	1079 C LEU 360	51.437 3.001 32.638 1.00 19.29	PROT
20	ATOM	1080 O LEU 360	50.319 2.802 33.102 1.00 27.53	PROT
	ATOM	1081 N SER 361	52.375 2.061 32.596 1.00 21.73	PROT
	ATOM	1082 CA SER 361	52.139 0.712 33.114 1.00 23.03	PROT
	ATOM	1083 CB SER 361	53.415 -0.130 33.027 1.00 25.89	PROT
	ATOM	1084 OG SER 361	53.645 -0.613 31.717 1.00 27.77	PROT
25	ATOM	1085 C SER 361	51.681 0.730 34.563 1.00 23.26	PROT
	ATOM	1086 O SER 361	50.720 0.046 34.929 1.00 18.73	PROT
	ATOM	1087 N SER 362	52.388 1.524 35.367 1.00 29.84	PROT
	ATOM	1088 CA SER 362	52.141 1.668 36.799 1.00 24.49	PROT
	ATOM	1089 CB SER 362	53.435 2.089 37.491 1.00 26.14	PROT
30	ATOM	1090 OG SER 362	53.917 3.305 36.949 1.00 25.03	PROT
	ATOM	1091 C SER 362	51.031 2.635 37.210 1.00 26.86	PROT
	ATOM	1092 O SER 362	50.797 2.831 38.404 1.00 39.63	PROT
	ATOM	1093 N PHE 363	50.361 3.251 36.240 1.00 20.94	PROT
	ATOM	1094 CA PHE 363	49.272 4.185 36.545 1.00 18.33	PROT
35	ATOM	1095 CB PHE 363	49.191 5.294 35.486 1.00 17.03	PROT
	ATOM	1096 CG PHE 363	50.171 6.407 35.706 1.00 22.73	PROT
	ATOM	1097 CD1 PHE 363	49.733 7.689 35.990 1.00 9.72	PROT
	ATOM	1098 CD2 PHE 363	51.545 6.167 35.659 1.00 24.77	PROT
	ATOM	1099 CE1 PHE 363	50.645 8.712 36.225 1.00 16.85	PROT
40	ATOM	1100 CE2 PHE 363	52.463 7.198 35.897 1.00 14.26	PROT
	ATOM	1101 CZ PHE 363	52.011 8.462 36.179 1.00 2.26	PROT
	ATOM	1102 C PHE 363	47.958 3.417 36.598 1.00 16.57	PROT
	ATOM	1103 O PHE 363	46.971 3.882 37.165 1.00 13.08	PROT
	ATOM	1104 N ASN 364	47.976 2.231 36.002 1.00 17.31	PROT
45	ATOM	1105 CA ASN 364	46.819 1.349 35.949 1.00 26.11	PROT
	ATOM	1106 CB ASN 364	46.673 0.608 37.276 1.00 16.96	PROT
	ATOM	1107 CG ASN 364	47.402 -0.715 37.267 1.00 31.34	PROT
	ATOM	1108 OD1 ASN 364	46.965 -1.657 36.613 1.00 36.66	PROT
	ATOM	1109 ND2 ASN 364	48.527 -0.794 37.985 1.00 31.61	PROT
50	ATOM	1110 C ASN 364	45.527 2.060 35.594 1.00 18.22	PROT

	A TON 4	1111 O ASN 364	44.522 1.923 36.286 1.00 23.17	PROT
	ATOM ATOM	1112 N LEU 365	45.567 2.803 34.491 1.00 13.10	PROT
	ATOM	1112 N EEU 305	44.417 3.562 34.013 1.00 15.41	PROT
	ATOM	1114 CB LEU 365	44.833 4.483 32.861 1.00 16.55	PROT
5	ATOM	1115 CG LEU 365	45.762 5.653 33.181 1.00 19.56	PROT
J	ATOM	1116 CD1 LEU 365	46.146 6.373 31.897 1.00 6.69	PROT
	ATOM	1117 CD2 LEU 365	45.067 6.602 34.128 1.00 15.69	PROT
	ATOM	1118 C LEU 365	43.328 2.624 33.520 1.00 12.07	PROT
	ATOM	1119 O LEU 365	43.620 1.534 33.043 1.00 19.81	PROT
10	ATOM	1119 O EEO 303 1120 N ASP 366	42.077 3.047 33.653 1.00 10.86	PROT
10	ATOM	1121 CA ASP 366	40.942 2.263 33.180 1.00 8.96	PROT
	ATOM	1122 CB ASP 366	39.933 2.021 34.326 1.00 9.59	PROT
	ATOM	1122 CB ASP 366	39.300 3.306 34.859 1.00 21.78	PROT
	ATOM	1124 OD1 ASP 366	39.871 4.397 34.676 1.00 25.60	PROT
15	ATOM	1125 OD2 ASP 366	38.217 3.222 35.474 1.00 19.16	PROT
13	ATOM	1126 C ASP 366	40.288 3.005 32.002 1.00 8.82	PROT
	ATOM	1127 O ASP 366	40.666 4.132 31.681 1.00 17.66	PROT
	ATOM	1128 N ASP 367	39.321 2.379 31.346 1.00 9.45	PROT
	ATOM	1129 CA ASP 367	38.668 3.023 30.218 1.00 11.11	PROT
20	ATOM	1130 CB ASP 367	37.457 2.205 29.769 1.00 20.67	PROT
	ATOM	1131 CG ASP 367	37.832 0.812 29.301 1.00 25.02	PROT
	ATOM	1132 OD1 ASP 367	39.040 0.525 29.158 1.00 21.06	PROT
	ATOM	1133 OD2 ASP 367	36.909 0.002 29.076 1.00 31.37	PROT
	ATOM	1134 C ASP 367	38.233 4.445 30.574 1.00 14.44	PROT
25	ATOM	1135 O ASP 367	38.457 5.380 29.815 1.00 26.42	PROT
	ATOM	1136 N THR 368	37.619 4.612 31.735 1.00 13.62	PROT
	ATOM	1137 CA THR 368	37.157 5.926 32.160 1.00 13.14	PROT
	ATOM	1138 CB THR 368	36.510 5.853 33.547 1.00 16.53	PROT
	ATOM	1139 OG1 THR 368	35.482 4.856 33.550 1.00 10.44	PROT
30	ATOM	1140 CG2 THR 368	35.928 7.188 33.925 1.00 5.20	PROT
	ATOM	1141 C THR 368	38.291 6.942 32.226 1.00 13.03	PROT
	ATOM	1142 O THR 368	38.114 8.108 31.878 1.00 12.90	PROT
	ATOM	1143 N GLU 369	39.455 6.492 32.686 1.00 9.96	PROT
	ATOM	1144 CA GLU 369	40.616 7.365 32.821 1.00 7.34	PROT
35	ATOM	1145 CB GLU 369	41.673 6.687 33.708 1.00 10.25	PROT
	ATOM	1146 CG GLU 369	41.584 7.113 35.189 1.00 14.56	PROT
	ATOM	1147 CD GLU 369	41.599 5.945 36.167 1.00 19.39	PROT
	ATOM	1148 OE1 GLU 369	42.255 4.922 35.864 1.00 19.65	PROT
	ATOM	1149 OE2 GLU 369	40.954 6.054 37.233 1.00 7.98	PROT
40		1150 C GLU 369	41.203 7.768 31.468 1.00 4.33	PROT
	ATOM	1151 O GLU 369	41.467 8.944 31.213 1.00 7.50	PROT
	ATOM	1152 N VAL 370	41.406 6.784 30.603 1.00 12.29	PROT
	ATOM	1153 CA VAL 370	41.927 7.040 29.267 1.00 19.01	PROT
	ATOM	1154 CB VAL 370	42.092 5.726 28.496 1.00 10.10	PROT
45	ATOM	1155 CG1 VAL 370	42.431 6.011 27.049 1.00 8.57	PROT
	ATOM	1156 CG2 VAL 370	43.168 4.877 29.159 1.00 12.40	PROT
	ATOM	1157 C VAL 370	40.896 7.915 28.555 1.00 18.30	PROT
•	ATOM	1158 O VAL 370	41.230 8.872 27.855 1.00 17.19	PROT
50	ATOM	1159 N ALA 371	39.633 7.581 28.760 1.00 2.00	PROT
50	ATOM	1160 CA ALA 371	38.549 8.321 28.157 1.00 3.53	PROT

	ATOM	1161 CB ALA 371	37.215 7.728 28.591 1.00 9.17	PROT
	ATOM	1162 C ALA 371	38.603 9.797 28.529 1.00 9.97	PROT
	ATOM	1163 O ALA 371	38.626 10.666 27.655 1.00 24.55	PROT
	ATOM	1164 N LEU 372	38.633 10.082 29.831 1.00 14.85	PROT
5	ATOM	1165 CA LEU 372	38.636 11.463 30.307 1.00 9.24	PROT
	ATOM	1166 CB LEU 372	38.480 11.501 31.830 1.00 8.83	PROT
	ATOM	1167 CG LEU 372	37.043 11.288 32.364 1.00 5.50	PROT
	ATOM	1168 CD1 LEU 372	37.036 10.338 33.553 1.00 2.02	PROT
	ATOM	1169 CD2 LEU 372	36.455 12.626 32.770 1.00 2.00	PROT
10	ATOM	1170 C LEU 372	39.867 12.218 29.870 1.00 10.17	PROT
	ATOM	1171 O LEU 372	39.791 13.413 29.568 1.00 7.23	PROT
	ATOM	1172 N LEU 373	40.996 11.510 29.825 1.00 13.10	PROT
	ATOM	1173 CA LEU 373	42.270 12.078 29.399 1.00 2.00	PROT
	ATOM	1174 CB LEU 373	43.325 10.981 29.381 1.00 2.00	PROT
15	ATOM		44.705 11.118 30.045 1.00 9.64	PROT
	ATOM	1176 CD1 LEU 373	44.817 12.382 30.875 1.00 2.00	PROT
	ATOM	1177 CD2 LEU 373	44.955 9.883 30.882 1.00 2.00	PROT
	ATOM	1178 C LEU 373	42.026 12.602 27.987 1.00 6.58	PROT
	ATOM	1179 O LEU 373	42.357 13.738 27.660 1.00 9.73	PROT
20	ATOM	1180 N GLN 374	41.401 11.763 27.165 1.00 9.45	PROT
	ATOM	1181 CA GLN 374	41.076 12.097 25.785 1.00 2.00	PROT
	ATOM		40.382 10.914 25.121 1.00 2.00	PROT
	ATOM		41.332 9.896 24.537 1.00 2.00	PROT
	ATOM		40.630 8.641 24.095 1.00 2.00	PROT
25	ATOM	1185 OE1 GLN 374	41.261 7.622 23.855 1.00 8.01	PROT
	ATOM	1186 NE2 GLN 374	39.316 8.705 23.989 1.00 2.00	PROT
	ATOM	1187 C GLN 374	40.187 13.326 25.694 1.00 2.78	PROT
	ATOM	1188 O GLN 374	40.427 14.213 24.875 1.00 13.91	PROT
30	ATOM	1189 N ALA 375	39.151 13.386 26.521 1.00 2.00	PROT
30	ATOM	1190 CA ALA 375	38.261 14.546 26.505 1.00 2.00	PROT
	ATOM	1191 CB ALA 375	37.128 14.348 27.489 1.00 3.97	PROT
	ATOM	1192 C ALA 375	39.061 15.801 26.868 1.00 4.60	PROT
	ATOM	1193 O ALA 375	38.881 16.864 26.274 1.00 8.82	PROT
35	ATOM	1194 N VAL 376	39.956 15.667 27.842 1.00 9.01 40.772 16.790 28.267 1.00 7.36	PROT
33	ATOM ATOM	1195 CA VAL 376 1196 CB VAL 376	41.669 16.401 29.467 1.00 7.30	PROT PROT
	ATOM	1190 CB VAL 376	42.597 17.532 29.839 1.00 2.00	PROT
	ATOM	1198 CG2 VAL 376	40.801 16.076 30.646 1.00 9.15	PROT
	ATOM	1199 C VAL 376	41.629 17.256 27.110 1.00 3.94	PROT
40			41.788 18.455 26.880 1.00 2.00	PROT
-10	ATOM	1200 O VAL 370	42.179 16.297 26.379 1.00 3.92	PROT
	ATOM	1202 CA LEU 377	43.020 16.618 25.239 1.00 5.65	PROT
	ATOM	1203 CB LEU 377	43.714 15.354 24.731 1.00 5.08	PROT
	ATOM	1204 CG LEU 377	45.052 15.005 25.386 1.00 2.00	PROT
45	ATOM	1205 CD1 LEU 377	45.620 13.790 24.719 1.00 2.00	PROT
	ATOM	1206 CD2 LEU 377	46.016 16.157 25.264 1.00 4.14	PROT
	ATOM	1207 C LEU 377	42.173 17.271 24.137 1.00 11.35	PROT
	ATOM	1208 O LEU 377	42.607 18.240 23.515 1.00 8.78	PROT
	ATOM	1209 N LEU 378	40.959 16.766 23.912 1.00 5.62	PROT
50	ATOM	1210 CA LEU 378	40.080 17.352 22.900 1.00 8.57	PROT

	ATOM	1211 CB LEU 378	38.784 16.553 22.788 1.00 5.98	PROT
	ATOM	1212 CG LEU 378	37.847 16.993 21.658 1.00 6.60	PROT
	ATOM	1213 CD1 LEU 378	38.550 16.826 20.329 1.00 2.00	PROT
	ATOM	1214 CD2 LEU 378	36.563 16.172 21.690 1.00 9.27	PROT
5	ATOM	1215 C LEU 378	39.738 18.833 23.146 1.00 10.76	PROT
	ATOM	1216 O LEU 378	40.045 19.689 22.312 1.00 14.81	PROT
	ATOM	1217 N MET 379	39.106 19.139 24.278 1.00 13.15	PROT
	ATOM	1218 CA MET 379	38.735 20.521 24.591 1.00 13.60	PROT
	ATOM	1219 CB MET 379	37.698 20.543 25.709 1.00 12.57	PROT
10	ATOM	1220 CG MET 379	36.425 19.782 25.395 1.00 21.12	PROT
	ATOM	1221 SD MET 379	35.533 20.396 23.927 1.00 15.79	PROT
	ATOM	1222 CE MET 379	34.397 19.099 23.756 1.00 13.95	PROT
	ATOM	1223 C MET 379	39.912 21.419 24.988 1.00 16.01	PROT
	ATOM	1224 O MET 379	39.981 21.897 26.121 1.00 16.95	PROT
15	ATOM	1225 N SER 380	40.824 21.663 24.048 1.00 12.39	PROT
	ATOM	1226 CA SER 380	41.984 22.506 24.303 1.00 10.77	PROT
	ATOM	1227 CB SER 380	43.248 21.815 23.810 1.00 8.45	PROT
	ATOM	1228 OG SER 380	43.288 20.487 24.286 1.00 17.27	PROT
	ATOM	1229 C SER 380	41.825 23.859 23.621 1.00 15.58	PROT
20	ATOM	1230 O SER 380	42.125 24.019 22.432 1.00 23.09	PROT
	ATOM	1231 N SER 381	41.368 24.837 24.396 1.00 23.65	PROT
	ATOM	1232 CA SER 381	41.123 26.187 23.904 1.00 25.18	PROT
	ATOM	1233 CB SER 381	40.449 27.018 25.003 1.00 34.78	PROT
	ATOM	1234 OG SER 381	41.250 27.073 26.170 1.00 37.79	PROT
25	ATOM	1235 C SER 381	42.342 26.940 23.388 1.00 19.38	PROT
	ATOM	1236 O SER 381	42.216 28.032 22.850 1.00 28.81	PROT
	ATOM	1237 N ASP 382	43.519 26.361 23.523 1.00 11.80	PROT
	ATOM	1238 CA ASP 382	44.716 27.057 23.082 1.00 15.78	PROT
	ATOM	1239 CB ASP 382	45.908 26.595 23.909 1.00 33.97	PROT
30	ATOM	1240 CG ASP 382	46.069 25.098 23.891 1.00 48.78	PROT
	ATOM	1241 OD1 ASP 382	45.169 24.401 24.406 1.00 45.58	PROT
	ATOM	1242 OD2 ASP 382	47.091 24.620 23.356 1.00 56.52	PROT
	ATOM	1243 C ASP 382	45.037 26.888 21.604 1.00 21.28	PROT
	ATOM	1244 O ASP 382	45.907 27.585 21.079 1.00 41.91	PROT
35	ATOM	1245 N ARG 383	44.357 25.971 20.923 1.00 21.81	PROT
	ATOM	1246 CA ARG 383	44.636 25.773 19.503 1.00 18.95	PROT
	ATOM	1247 CB ARG 383	43.745 24.685 18.921 1.00 8.26	PROT
	ATOM	1248 CG ARG 383	43.580 23.491 19.821 1.00 18.07	PROT
	ATOM	1249 CD ARG 383	44.693 22.487 19.610 1.00 11.10	PROT
40	ATOM	1250 NE ARG 383	44.480 21.261 20.378 1.00 20.54	PROT
	ATOM	1251 CZ ARG 383	45.460 20.462 20.786 1.00 18.25	PROT
	ATOM	1252 NH1 ARG 383	45.187 19.365 21.481 1.00 5.24	PROT
	ATOM	1253 NH2 ARG 383	46.717 20.765 20.495 1.00 19.21	PROT
	ATOM	1254 C ARG 383	44.420 27.064 18.728 1.00 19.64	PROT
45	ATOM	1255 O ARG 383	43.493 27.828 19.001 1.00 17.46	PROT
	ATOM	1256 N PRO 384	45.298 27.342 17.762 1.00 25.37	PROT
	ATOM	1257 CD PRO 384	46.485 26.567 17.359 1.00 35.06	PROT
	ATOM	1258 CA PRO 384	45.124 28.569 16.983 1.00 27.53	PROT
	ATOM	1259 CB PRO 384	46.422 28.693 16.181 1.00 18.75	PROT
50	ATOM	1260 CG PRO 384	47.041 27.338 16.190 1.00 27.78	PROT

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	A T/ON 4	1261 C PRO 384	43.895 28.476 16.081 1.00 28.76	PROT
	ATOM	1261 C PRO 384 1262 O PRO 384	43.562 27.402 15.560 1.00 31.18	PROT
	ATOM		43.215 29.606 15.917 1.00 27.37	PROT
	ATOM		42.039 29.638 15.073 1.00 26.98	PROT
_	ATOM		42.039 29.038 15.073 1.00 20.98	PROT
5	ATOM		39.689 29.911 15.339 1.00 31.99	PROT
	ATOM		40.756 28.756 16.939 1.00 31.99	PROT
	ATOM			PROT
	ATOM	1268 CA LEU 386	39.524 28.515 17.673 1.00 37.24	
10	ATOM	1269 CB LEU 386	39.820 27.947 19.059 1.00 26.60	PROT PROT
10	ATOM	1270 CG LEU 386	40.233 26.472 18.988 1.00 32.45	
	ATOM	1271 CD1 LEU 386	40.177 25.859 20.363 1.00 34.82	PROT
	ATOM	1272 CD2 LEU 386	39.314 25.719 18.030 1.00 29.64	PROT
	ATOM	1273 C LEU 386	38.733 29.795 17.778 1.00 36.93	PROT
	ATOM	1274 O LEU 386	39.291 30.881 17.674 1.00 37.60	PROT
15	ATOM	1275 N ALA 387	37.427 29.665 17.962 1.00 31.47	PROT
	ATOM	1276 CA ALA 387	36.578 30.832 18.058 1.00 28.80	PROT
	ATOM	1277 CB ALA 387	35.553 30.814 16.950 1.00 41.01	PROT
	ATOM	1278 C ALA 387	35.890 30.864 19.400 1.00 28.89	PROT
	ATOM	1279 O ALA 387	35.998 31.842 20.133 1.00 30.62	PROT
20	ATOM	1280 N CYS 388	35.167 -29.797 19.710 1.00 25.92	PROT
	ATOM	1281 CA CYS 388	34.469 29.712 20.978 1.00 26.90	PROT
	ATOM	1282 CB CYS 388	33.224 28.823 20.826 1.00 21.38	PROT
	ATOM	1283 SG CYS 388	31.625 29.732 20.698 1.00 33.66	PROT
	ATOM	1284 C CYS 388	35.443 29.159 22.040 1.00 31.18	PROT
25	ATOM	1285 O CYS 388	35.272 28.054 22.552 1.00 36.57	PROT
	ATOM	1286 N VAL 389	36.473 29.951 22.346 1.00 20.22	PROT
	ATOM	1287 CA VAL 389	37.511 29.622 23.327 1.00 16.02	PROT
	ATOM	1288 CB VAL 389	38.554 30.737 23.381 1.00 9.80	PROT
	ATOM	1289 CG1 VAL 389	39.526 30.480 24.498 1.00 16.03	PROT
30	ATOM	1290 CG2 VAL 389	39.257 30.843 22.056 1.00 16.27	PROT
	ATOM	1291 C VAL 389	36.977 29.425 24.753 1.00 18.85	PROT
	ATOM	1292 O VAL 389	37.066 28.336 25.323 1.00 24.21	PROT
	ATOM	1293 N GLU 390	36.461 30.500 25.337 1.00 5.06	PROT
	ATOM	1294 CA GLU 390	35.908 30.434 26.660 1.00 2.00	PROT
35	ATOM	1295 CB GLU 390	35.092 31.684 26.952 1.00 5.13	PROT
	ATOM	1296 C GLU 390	35.047 29.184 26.817 1.00 3.75	PROT
	ATOM	1297 O GLU 390	35.252 28.419 27.754 1.00 23.35	PROT
	ATOM	1298 N ARG 391	34.103 28.938 25.915 1.00 14.06	PROT
	ATOM	1299 CA ARG 391	33.248 27.754 26.093 1.00 26.18	PROT
40	ATOM	1300 CB ARG 391	32.121 27.699 25.049 1.00 31.84	PROT
	ATOM	1301 CG ARG 391	30.843 27.040 25.601 1.00 47.73	PROT
	ATOM	1302 CD ARG 391	29.882 26.572 24.512 1.00 58.24	PROT
	ATOM	1303 NE ARG 391	29.879 27.487 23.378 1.00 66.80	PROT
	ATOM	1304 CZ ARG 391	29.001 28.470 23.211 1.00 69.56	PROT
45	ATOM	1305 NH1 ARG 391	29.088 29.255 22.139 1.00 66.99	PROT
	ATOM	1306 NH2 ARG 391	28.034 28.663 24.105 1.00 56.08	PROT
	ATOM	1307 C ARG 391	33.979 26.415 26.110 1.00 23.65	PROT
	ATOM	1308 O ARG 391	33.561 25.479 26.794 1.00 28.58	PROT
	ATOM	1309 N ILE 392	35.064 26.316 25.359 1.00 15.05	PROT
50	ATOM	1310 CA ILE 392	35.812 25.077 25.335 1.00 19.03	PROT

	ATOM	1311 CB ILE 392	36.804 25.063 24.165 1.00 22.30	PROT
	ATOM	1312 CG2 ILE 392	37.971 24.130 24.467 1.00 21.71	PROT
	ATOM	1313 CG1 ILE 392	36.074 24.614 22.892 1.00 23.47	PROT
	ATOM	1314 CD1 ILE 392	36.245 25.551 21.707 1.00 4.13	PROT
5	ATOM	1315 C ILE 392	36.544 24.907 26.671 1.00 25.03	PROT
	ATOM	1316 O ILE 392	36.728 23.783 27.153 1.00 26.11	PROT
	ATOM	1317 N GLU 393	36.947 26.029 27.266 1.00 30.74	PROT
	ATOM	1318 CA GLU 393	37.630 26.021 28.558 1.00 23.39	PROT
	ATOM	1319 CB GLU 393	38.073 27.430 28.930 1.00 27.18	PROT
10	ATOM	1320 CG GLU 393	39.435 27.817 28.402 1.00 41.39	PROT
	ATOM	1321 CD GLU 393	39.990 29.051 29.093 1.00 47.72	PROT
	ATOM	1322 OE1 GLU 393	39.365 29.524 30.070 1.00 39.94	PROT
	ATOM	1323 OE2 GLU 393	41.051 29.547 28.653 1.00 51.17	PROT
	ATOM	1324 C GLU 393	36.655 25.516 29.610 1.00 21.72	PROT
15	ATOM	1325 O GLU 393	36.942 24.574 30.344 1.00 22.82	PROT
	ATOM	1326 N LYS 394	35.497 26.163 29.676 1.00 9.64	PROT
	ATOM	1327 CA LYS 394	34.462 25.779 30.618 1.00 11.56	PROT
	ATOM	1328 CB LYS 394	33.177 26.557 30.338 1.00 7.52	PROT
	ATOM	1329 C LYS 394	34.213 24.280 30.492 1.00 16.31	PROT
20	ATOM	1330 O LYS 394	34.000 23.594 31.498 1.00 24.52	PROT
	ATOM	1331 N TYR 395	34.251 23.763 29.264 1.00 12.79	PROT
	ATOM	1332 CA TYR 395	34.033 22.332 29.057 1.00 19.02	PROT
	ATOM	1333 CB TYR 395	33.803 22.025 27.572 1.00 27.90	PROT
	ATOM	1334 CG TYR 395	32.454 22.456 27.027 1.00 31.64	PROT
25	ATOM	1335 CD1 TYR 395	32.136 22.267 25.684 1.00 30.15	PROT
	ATOM	1336 CE1 TYR 395	30.927 22.695 25.160 1.00 28.34	PROT
	ATOM	1337 CD2 TYR 395	31.514 23.085 27.835 1.00 34.21	PROT
	ATOM	1338 CE2 TYR 395	30.298 23.518 27.317 1.00 34.01	PROT
	ATOM	1339 CZ TYR 395	30.014 23.322 25.979 1.00 33.73	PROT
30	ATOM	1340 OH TYR 395	28.824 23.785 25.453 1.00 44.99	PROT
	ATOM	1341 C TYR 395	35.208 21.490 29.584 1.00 19.03	PROT
	ATOM	1342 O TYR 395	35.003 20.494 30.277 1.00 25.23	PROT
	ATOM	1343 N GLN 396	36.437 21.883 29.256 1.00 17.76	PROT
	ATOM	1344 CA GLN 396	37.596 21.134 29.725 1.00 13.73	PROT
35	ATOM	1345 CB GLN 396	38.905 21.766 29.240 1.00 2.45	PROT
	ATOM	1346 CG GLN 396	40.061 20.767 29.110 1.00 2.00	PROT
	ATOM	1347 CD GLN 396	41.388 21.439 28.799 1.00 5.12 41.706 22.484 29.359 1.00 10.11	PROT PROT
	ATOM	1348 OE1 GLN 396	42.169 20.840 27.903 1.00 9.09	PROT
40	ATOM	1349 NE2 GLN 396		
40	ATOM	1350 C GLN 396 1351 O GLN 396	37.562 21.149 31.238 1.00 17.65 37.802 20.125 31.894 1.00 9.63	PROT PROT
	ATOM		37.802 20.123 31.894 1.00 9.03 37.250 22.319 31.787 1.00 6.69	PROT
	ATOM	1352 N ASP 397 1353 CA ASP 397	37.178 22.476 33.226 1.00 9.36	PROT
	ATOM	1354 CB ASP 397	36.732 23.893 33.570 1.00 11.44	PROT
15	ATOM	1355 CG ASP 397	37.867 24.891 33.446 1.00 18.32	PROT
45	ATOM ATOM	1356 OD1 ASP 397	39.033 24.438 33.397 1.00 24.00	PROT
	ATOM	1357 OD2 ASP 397	37.615 26.114 33.395 1.00 20.67	PROT
	ATOM	1358 C ASP 397	36.215 21.443 33.771 1.00 7.77	PROT
	ATOM	1359 O ASP 397	36.497 20.771 34.761 1.00 7.66	PROT
50	ATOM	1360 N SER 398	35.087 21.293 33.093 1.00 9.19	PROT
20	7 1 4 O 141	.550 II DER 570		1

	ATOM	1361 CA SER 398	34.094 20.322 33.508 1.00 14.18	PROT
	ATOM	1362 CB SER 398	32.916 20.334 32.542 1.00 12.11	PROT
	ATOM	1363 OG SER 398	32.406 21.650 32.423 1.00 31.95	PROT
	ATOM	1364 C SER 398	34.712 18.939 33.556 1.00 11.47	PROT
5	ATOM	1365 O SER 398	34.591 18.227 34.551 1.00 21.11	PROT
	ATOM	1366 N PHE 399	35.394 18.565 32.485 1.00 18.68	PROT
	ATOM	1367 CA PHE 399	36.017 17.252 32.417 1.00 24.93	PROT
	ATOM	1368 CB PHE 399	36.587 17.012 31.014 1.00 23.38	PROT
	ATOM	1369 CG PHE 399	35.543 16.705 29.981 1.00 20.19	PROT
10	ATOM	1370 CD1 PHE 399	35.224 17.638 28.997 1.00 22.94	PROT
	ATOM	1371 CD2 PHE 399	34.878 15.486 29.988 1.00 8.62	PROT
	ATOM	1372 CE1 PHE 399	34.257 17.361 28.029 1.00 12.53	PROT
	ATOM	1373 CE2 PHE 399	33.914 15.201 29.027 1.00 19.25	PROT
	ATOM	1374 CZ PHE 399	33.604 16.143 28.044 1.00 15.15	PROT
15	ATOM	1375 C PHE 399	37.113 17.097 33.463 1.00 23.06	PROT
	ATOM	1376 O PHE 399	37.210 16.063 34.137 1.00 15.58	PROT
	ATOM	1377 N LEU 400	37.932 18.131 33.604 1.00 22.12	PROT
	ATOM	1378 CA LEU 400	39.017 18.095 34.567 1.00 18.27	PROT
	ATOM	1379 CB LEU 400	39.846 19.372 34.461 1.00 10.06	PROT
20	ATOM	1380 CG LEU 400	41.021 19.248 33.491 1.00 8.13	PROT
	ATOM	1381 CD1 LEU 400	41.616 20.594 33.195 1.00 2.00	PROT
	ATOM	1382 CD2 LEU 400	42.055 18.333 34.095 1.00 13.73	PROT
	ATOM	1383 C LEU 400	38.527 17.892 36.002 1.00 24.79	PROT
	ATOM	1384 O LEU 400	39.189 17.228 36.787 1.00 26.46	PROT
25	ATOM	1385 N LEU 401	37.371 18.447 36.354 1.00 21.93	PROT
	ATOM	1386 CA LEU 401	36.862 18.268 37.707 1.00 17.21	PROT
	ATOM	1387 CB LEU 401	35.766 19.285 38.022 1.00 19.27	PROT
	ATOM	1388 CG LEU 401	35.538 19.547 39.515 1.00 16.76	PROT
	ATOM	1389 CD1 LEU 401	36.652 20.403 40.085 1.00 2.00	PROT
30	ATOM	1390 CD2 LEU 401	34.206 20.235 39.687 1.00 14.41	PROT
	ATOM	1391 C LEU 401	36.316 16.864 37.879 1.00 18.03	PROT
	ATOM	1392 O LEU 401	36.482 16.250 38.925 1.00 28.63	PROT
	ATOM	1393 N ALA 402	35.656 16.346 36.856 1.00 9.30	PROT
	ATOM	1394 CA ALA 402	35.124 15.000 36.951 1.00 7.03	PROT
35	ATOM	1395 CB ALA 402	34.233 14.703 35.758 1.00 14.15	PROT
	ATOM	1396 C ALA 402	36.298 14.029 36.989 1.00 7.68	PROT
	ATOM	1397 O ALA 402	36.294 13.054 37.739 1.00 2.00	PROT
	ATOM	1398 N PHE 403	37.311 14.305 36.178 1.00 4.49	PROT
	ATOM	1399 CA PHE 403	38.477 13.439 36.140 1.00 9.18	PROT
40	ATOM	1400 CB PHE 403	39.510 13.977 35.138 1.00 12.80	PROT
	ATOM	1401 CG PHE 403	40.545 12.957 34.693 1.00 5.42	PROT
	ATOM	1402 CD1 PHE 403	41.590 13.334 33.859 1.00 2.00	PROT
	ATOM	1403 CD2 PHE 403	40.480 11.634 35.103 1.00 2.00	PROT
	ATOM	1404 CE1 PHE 403	42.546 12.410 33.448 1.00 2.00	PROT
45	ATOM	1405 CE2 PHE 403	41.440 10.711 34.688 1.00 2.00	PROT
	ATOM	1406 CZ PHE 403	42.468 11.100 33.863 1.00 2.00	PROT
	ATOM	1407 C PHE 403	39.080 13.366 37.539 1.00 10.08	PROT
	ATOM	1408 O PHE 403	39.207 12.279 38.097 1.00 8.23	PROT
	ATOM	1409 N GLU 404	39.451 14.514 38.103 1.00 12.64	PROT
50	ATOM	1410 CA GLU 404	40.030 14.546 39.448 1.00 19.23	PROT

	ATOM	1411 CB GLU 404 40.227 15.989 39.942 1.00 19.80 PROT
	ATOM	1412 CG GLU 404 41.532 16.220 40.728 1.00 24.03 PROT
	ATOM	1413 CD GLU 404 41.474 17.429 41.655 1.00 29.60 PROT
	ATOM	1414 OE1 GLU 404 41.706 18.565 41.182 1.00 29.51 PROT
5	ATOM	1415 OE2 GLU 404 41.197 17.247 42.861 1.00 30.42 PROT
	ATOM	1416 C GLU 404 39.112 13.806 40.416 1.00 24.36 PROT
	ATOM	1417 O GLU 404 39.571 12.963 41.200 1.00 28.04 PROT
	ATOM	1418 N HIS 405 37.815 14.108 40.358 1.00 10.26 PROT
	ATOM	1419 CA HIS 405 36.870 13.446 41.240 1.00 7.78 PROT
10	ATOM	1420 CB HIS 405 35.473 14.023 41.054 1.00 3.47 PROT
	ATOM	1421 CG HIS 405 35.312 15.393 41.630 1.00 15.49 PROT
	ATOM	1422 CD2 HIS 405 36.223 16.260 42.134 1.00 17.97 PROT
	ATOM	1423 ND1 HIS 405 34.096 16.036 41.694 1.00 21.57 PROT
	ATOM	1424 CE1 HIS 405 34.265 17.242 42.210 1.00 27.50 PROT
15	ATOM	1425 NE2 HIS 405 35.547 17.403 42.485 1.00 13.53 PROT
	ATOM	1426 C HIS 405 36.856 11.936 41.005 1.00 14.88 PROT
	ATOM	1427 O HIS 405 36.641 11.155 41.935 1.00 22.11 PROT
	ATOM	1428 N TYR 406 37.091 11.512 39.767 1.00 16.52 PROT
	ATOM	1429 CA TYR 406 37.085 10.083 39.491 1.00 14.35 PROT
20	ATOM	1430 CB TYR 406 37.007 9.808 37.989 1.00 9.90 PROT
	ATOM	1431 CG TYR 406 36.840 8.346 37.657 1.00 2.00 PROT
	ATOM	1432 CD1 TYR 406 35.587 7.742 37.676 1.00 8.84 PROT
	ATOM	1433 CE1 TYR 406 35.433 6.382 37.386 1.00 8.78 PROT
	ATOM	1434 CD2 TYR 406 37.939 7.562 37.338 1.00 15.34 PROT
25	ATOM	1435 CE2 TYR 406 37.801 6.204 37.044 1.00 13.48 PROT
	ATOM	1436 CZ TYR 406 36.548 5.624 37.073 1.00 15.64 PROT
	ATOM	1437 OH TYR 406 36.431 4.287 36.804 1.00 2.00 PROT
	ATOM	1438 C TYR 406 38.340 9.466 40.071 1.00 9.54 PROT
	ATOM	1439 O TYR 406 38.328 8.328 40.525 1.00 14.29 PROT
30	ATOM	1440 N ILE 407 39.430 10.217 40.058 1.00 6.56 PROT
	ATOM	1441 CA ILE 407 40.671 9.708 40.617 1.00 13.87 PROT
	ATOM	1442 CB ILE 407 41.808 10.728 40.474 1.00 11.28 PROT
	ATOM	1443 CG2 ILE 407 42.902 10.413 41.461 1.00 6.25 PROT
	ATOM	1444 CG1 ILE 407 42.357 10.714 39.039 1.00 18.73 PROT
35	ATOM	1445 CD1 ILE 407 41.863 9.579 38.169 1.00 13.14 PROT
	ATOM	1446 C ILE 407 40.438 9.426 42.091 1.00 11.44 PROT
	ATOM	1447 O ILE 407 40.691 8.325 42.571 1.00 4.46 PROT
	ATOM	1448 N ASN 408 39.953 10.448 42.792 1.00 12.35 PROT
	ATOM	1449 CA ASN 408 39.642 10.363 44.213 1.00 2.00 PROT
40	ATOM	1450 CB ASN 408 38.758 11.535 44.629 1.00 2.00 PROT
	ATOM	1451 CG ASN 408 39.499 12.840 44.657 1.00 3.57 PROT
		1452 OD1 ASN 408 40.733 12.859 44.656 1.00 14.35 PROT
		1453 ND2 ASN 408 38.758 13.949 44.689 1.00 2.00 PROT
		1454 C ASN 408 38.868 9.078 44.432 1.00 6.49 PROT
45		1455 O ASN 408 39.282 8.187 45.178 1.00 10.45 PROT
. =		1456 N TYR 409 37.731 8.987 43.766 1.00 2.00 PROT
		1457 CA TYR 409 36.900 7.816 43.893 1.00 9.20 PROT
		1458 CB TYR 409 35.879 7.783 42.760 1.00 11.66 PROT
		1459 CG TYR 409 35.121 6.489 42.683 1.00 12.54 PROT
50	ATOM	1460 CD1 TYR 409 33.984 6.281 43.456 1.00 29.23 PROT

ATOM 1462 CD2 TYR 409 35.547 5.465 41.850 1.00 24.96 PATOM 1463 CE2 TYR 409 34.860 4.259 41.788 1.00 33.40 PATOM 1464 CZ TYR 409 33.065 2.883 42.509 1.00 32.72 PATOM 1465 OH TYR 409 37.753 6.553 43.867 1.00 12.72 PATOM 1466 C TYR 409 37.753 6.553 43.867 1.00 13.96 PATOM 1468 N ARG 410 38.931 6.399 42.803 1.00 23.04 PATOM 1468 N ARG 410 39.977 5.230 42.588 1.00 22.09 PATOM 1470 CB ARG 410 38.937 5.230 42.588 1.00 22.09 PATOM 1471 CG ARG 410 38.934 4.111 39.275 1.00 16.49 PATOM 1472 CD ARG 410 38.934 4.111 39.275 1.00 16.49 PATOM 1473 NE ARG 410 40.227 3.848 38.651 1.00 9.77 PATOM 1473 NE ARG 410 40.617 2.651 38.239 1.00 11.38 PATOM 1475 NH1 ARG 410 40.617 2.651 38.239 1.00 11.38 PATOM 1476 NH2 ARG 410 40.860 3.753 43.780 1.00 12.78 PATOM 1478 O ARG 410 40.866 3.753 43.780 1.00 12.85 PATOM 1481 CB LYS 411 41.022 5.931 44.262 1.00 24.16 PATOM 1483 CD LYS 411 41.022 5.931 44.262 1.00 24.16 PATOM 1483 CD LYS 411 41.023 5.931 44.262 1.00 24.16 PATOM 1483 CD LYS 411 41.023 5.931 44.262 1.00 24.16 PATOM 1488 N HIS 412 44.091 5.438 43.923 1.00 10.83 PATOM 1488 N HIS 412 44.091 5.438 43.923 1.00 20.00 PATOM 1489 CA HIS 411 43.864 4.914 44.664 1.00 28.02 PATOM 1489 CA HIS 412 44.915 5.289 40.857 1.00 18.44 PATOM 1486 C LYS 411 43.186 4.814 44.664 1.00 28.02 PATOM 1489 CA HIS 412 44.915 5.438 43.923 1.00 30.05 PATOM 1489 CA HIS 412 44.915 5.438 43.923 1.00 20.00 PATOM 1489 CA HIS 412 45.262 4.738 43.332 1.00 20.00 PATOM 1490 CB HIS 412 45.566 4.465 39.833 1.00 16.33 PATOM 1490 CB HIS 412 45.366 4.465 39.833 1.00 16.33 PATOM 1491 CG HIS 412 45.366 4.465 39.833 1.00 16.33 PATOM 1493 NDI HIS 412 45.366 4.465 39.833 1.00 16.33 PATOM 1494 CEI HIS 412 45.366 4.465 39.833 1.00 16.33 PATOM 1498 N HIS 413 46.214 2.902 47.600 1.00 42.00 PATOM 1498 N HIS 413 46.906 2.053 46.759 1.00 44.26 PATOM 1499 CD HIS 413 46.916 2.053 46.759 1.00 44.26 PATOM 1490 CB HIS 413 46.910 2.015 46.281 47.98 47.900 1.00 40.00 PATOM 1500 CB HIS 413 46.910 2.010 47.35 PATOM 1500 CB HIS 413 46.910 2.010 47.35 PATOM 1500 CB HIS 413 46.010 2.01 47.35 PATOM 15	PROT
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45 ATOM 1505 NEGRIDO 410 45011 1107 47 200 1 00 2550 PD	PROT
45 ATOM 1505 NE2 HIS 413 45.011 1.137 47.390 1.00 35.50 PR	PROT
ATOM 1506 C HIS 413 49.527 4.194 44.875 1.00 26.49 PRC	PROT
ATOM 1507 O HIS 413 50.483 3.421 44.829 1.00 31.82 PRC	PROT
	PROT
	PROT
50 ATOM 1510 CB VAL 414 50.718 5.966 42.290 1.00 32.50 PF	PROT

	ATOM	1511 CG1 VAL 414 51.636 7.0	26 41.694 1.00 33.83	PROT
	ATOM		74 41.863 1.00 40.20	PROT
	ATOM		44.225 1.00 17.96	PROT
	ATOM		5 43.829 1.00 30.33	PROT
5	ATOM		45.028 1.00 32.51	PROT
,	ATOM		32 45,531 1.00 35.31	PROT
	ATOM		9 46.511 1.00 49.75	PROT
	ATOM		930 46.702 1.00 60.64	PROT
	ATOM		50 45.974 1.00 50.83	PROT
10	ATOM		7 44.436 1.00 31.44	PROT
	ATOM	1521 O THR 415 52.423 10.25	1 43.475 1.00 22.01	PROT
	ATOM		44.607 1.00 24.94	PROT
	ATOM		9 43.671 1.00 27.82	PROT
	ATOM		4 43.440 1.00 32.98	PROT
15	ATOM		7 44.671 1.00 44.74	PROT
	ATOM	1526 CD2 HIS 416 53.982 13.5	39 45.251 1.00 44.91	PROT
	ATOM		65 45.462 1.00 49.20	PROT
	ATOM		00 46.477 1.00 53.14	PROT
	ATOM		30 46.373 1.00 41.72	PROT
20	ATOM		42.328 1.00 29.13	PROT
	ATOM		41.286 1.00 37.24	PROT
	ATOM		1 42.350 1.00 18.38	PROT
	ATOM		67 41.115 1.00 16.08	PROT
	ATOM		29 41.407 1.00 17.89	PROT
25	ATOM		7 40.364 1.00 16.15	PROT
	ATOM		44 40.051 1.00 16.55	PROT
	ATOM		71 39.696 1.00 15.49	PROT
	ATOM		81 39.087 1.00 19.81	PROT
	ATOM		08 38.731 1.00 9.76	PROT
30	ATOM		4 38.427 1.00 5.25	PROT
	ATOM		0 40.187 1.00 14.51	PROT
	ATOM		9 39.081 1.00 18.44	PROT
	ATOM		0 40.640 1.00 21.08	PROT PROT
	ATOM		00 39.828 1.00 16.28	PROT
35	ATOM		32 40.659 1.00 15.19 46 39.802 1.00 16.60	PROT
	ATOM		39.802 1.00 10.00 369 38.710 1.00 21.85	PROT
	ATOM		57 38.118 1.00 22.53	PROT
	ATOM		38 38.170 1.00 16.42	PROT
40	ATOM		07 39.836 1.00 21.01	PROT
40	ATOM		506 38.826 1.00 24.02	PROT
	ATOM ATOM	1552 CZ2 TRP 418 42.838 16.5	55 37.010 1.00 24.64	PROT
	ATOM		35 37.069 1.00 28.80	PROT
	ATOM		337 36.500 1.00 21.25	PROT
45	ATOM		6 39.192 1.00 16.17	PROT
43	ATOM		4 37.977 1.00 19.51	PROT
	ATOM		60 40.007 1.00 19.59	PROT
	ATOM		74 41.477 1.00 19.81	PROT
	ATOM		02 39.429 1.00 17.87	PROT
50	ATOM		09 40.629 1.00 6.85	PROT

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49.785 16.326 41.764 1.00 25.11
                                                              PROT
    ATOM 1561 CG PRO 419
                              50.578 15.202 38.373 1.00 15.44
                                                             PROT
    ATOM 1562 C PRO 419
                                                             PROT
                              50.922 15.720 37.315 1.00 24.75
    ATOM 1563 O PRO 419
                              50.811 13.932 38.664 1.00 15.10
                                                             PROT
    ATOM 1564 N LYS 420
                               51.534 13.056 37.748 1.00 20.59
                                                             PROT
    ATOM 1565 CA LYS 420
                               51.900 11.746 38.471 1.00 28.85
                                                              PROT
     ATOM 1566 CB LYS 420
                               52.955 11.906 39.577 1.00 30.61
                                                              PROT
    ATOM 1567 CG LYS 420
    ATOM 1568 CD LYS 420
                               52.907 10.759 40.580 1.00 24.41
                                                              PROT
                               54.275 10.493 41.224 1.00 31.94
    ATOM 1569 CE LYS 420
                                                             PROT
    ATOM 1570 NZ LYS 420
                               54.485 9.040 41.557 1.00 27.34
                                                             PROT
10
    ATOM 1571 C LYS 420
                              50.779 12.757 36.445 1.00 17.36
                                                             PROT
    ATOM 1572 O LYS 420
                              51.393 12.439 35.437 1.00 26.28
                                                             PROT
                              49.455 12.859 36.474 1.00 16.34
                                                             PROT
     ATOM 1573 N LEU 421
                               48.627 12.614 35.297 1.00 9.38
                                                             PROT
    ATOM 1574 CA LEU 421
                               47.231 12.139 35.707 1.00 13.22
                                                              PROT
    ATOM 1575 CB LEU 421
15
                               46.739 10.818 35.107 1.00 15.75
                                                              PROT
     ATOM 1576 CG LEU 421
                                47.919 9.993 34.652 1.00 29.24
                                                              PROT
     ATOM 1577 CD1 LEU 421
                                45.949 10.049 36.135 1.00 12.19
                                                              PROT
     ATOM 1578 CD2 LEU 421
                              48.511 13.866 34.441 1.00 12.61
                                                             PROT
     ATOM 1579 C LEU 421
                              48.458 13.777 33.223 1.00 17.85
                                                             PROT
     ATOM 1580 O LEU 421
20
                               48.451 15.036 35.063 1.00 8.47
                                                             PROT
     ATOM 1581 N LEU 422
                               48.393 16.254 34.277 1.00 7.21
                                                             PROT
     ATOM 1582 CA LEU 422
                               48.160 17.468 35.164 1.00 2.00
                                                             PROT
     ATOM 1583 CB LEU 422
     ATOM 1584 CG LEU 422
                                46.941 17.445 36.088 1.00 12.16
                                                              PROT
     ATOM 1585 CD1 LEU 422
                                47.024 18.660 36.982 1.00 6.96
                                                              PROT
25
                                45.632 17.450 35.313 1.00 2.00
                                                              PROT
     ATOM 1586 CD2 LEU 422
                               49.748 16.365 33.567 1.00 10.59
                                                             PROT
     ATOM 1587 C LEU 422
                               49.851 16.938 32.477 1.00 13.48
                                                             PROT
     ATOM 1588 O LEU 422
                               50.786 15.804 34.185 1.00 2.29
                                                             PROT
     ATOM 1589 N MET 423
                                52.109 15.821 33.579 1.00 6.50
                                                              PROT
     ATOM 1590 CA MET 423
30
                                                              PROT
                                53.158 15.215 34.514 1.00 2.13
     ATOM 1591 CB MET 423
                                53.361 15.968 35.803 1.00 16.33
                                                              PROT
     ATOM 1592 CG MET 423
     ATOM 1593 SD MET 423
                                55.075 16.415 36.070 1.00 26.66
                                                              PROT
                                55.751 14.880 36.623 1.00 20.24
                                                              PROT
     ATOM 1594 CE MET 423
                               52.016 14.966 32.318 1.00 12.20
                                                             PROT
35
     ATOM 1595 C MET 423
                                                             PROT
                               52.741 15.183 31.345 1.00 18.67
     ATOM 1596 O MET 423
                               51.114 13.988 32.352 1.00 7.89
                                                             PROT
     ATOM 1597 N LYS 424
                                                              PROT
     ATOM 1598 CA LYS 424
                                50.907 13.084 31.230 1.00 12.91
                                                             PROT
     ATOM 1599 CB LYS 424
                               49.990 11.924 31.645 1.00 5.14
                                50,669 10,579 31.980 1.00 11.76
                                                              PROT
40
     ATOM 1600 CG LYS 424
     ATOM 1601 CD LYS 424
                                52.187 10.590 31.866 1.00 3.70
                                                              PROT
     ATOM 1602 CE LYS 424
                               52.844 10.020 33.113 1.00 7.84
                                                             PROT
                               54.335 9.959 32.995 1.00 25.86
                                                             PROT
     ATOM 1603 NZ LYS 424
                                                             PROT
     ATOM 1604 C LYS 424
                               50.293 13.840 30.046 1.00 17.44
     ATOM 1605 O LYS 424
                               50.650 13.596 28.897 1.00 11.72
                                                             PROT
45
     ATOM 1606 N VAL 425
                               49.370 14.756 30.322 1.00 3.16
                                                             PROT
                                48.768 15.515 29.249 1.00 2.00
                                                              PROT
     ATOM 1607 CA VAL 425
     ATOM 1608 CB VAL 425
                                47.744 16.532 29.773 1.00 6.77
                                                              PROT
     ATOM 1609 CG1 VAL 425
                                47.653 17.716 28.815 1.00 2.00
                                                              PROT
                                46.381 15.870 29.914 1.00 10.91
                                                              PROT
     ATOM 1610 CG2 VAL 425
50
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ATOM 1612 O VAL 425 ATOM 1613 N THR 426 ATOM 1614 CA THR 426 ATOM 1615 CB THR 426 ATOM 1616 OGI THR 426 ATOM 1617 CG2 THR 426 ATOM 1618 C THR 426 ATOM 1618 C THR 426 ATOM 1628 C ASP 427 ATOM 1620 N ASP 427 ATOM 1621 CA ASP 427 ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 OD1 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1628 N LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1634 C LEU 428 ATOM 1635 O LEU 428 ATOM 1635 O LEU 428 ATOM 1636 O ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1640 CD ARG 42		ATOM	1611 C VAL 425	49.845 16.274 28.487 1.00 4.83	PROT
ATOM 1614 CA THR 426 ATOM 1615 CB THR 426 ATOM 1615 CG THR 426 ATOM 1616 COG1 THR 426 ATOM 1617 CG2 THR 426 ATOM 1618 C THR 426 ATOM 1619 O THR 426 ATOM 1619 O THR 426 ATOM 1620 N ASP 427 ATOM 1621 CA ASP 427 ATOM 1622 CB ASP 427 ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 OD1 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1627 O ASP 427 ATOM 1630 CB LEU 428 ATOM 1630 CD LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1634 C LEU 428 ATOM 1635 O LEU 428 ATOM 1636 N ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1648 CA MET 430 ATOM 1655 N ILE 431 ATOM 1655 CG ILE 431 ATOM 1656 CA ILE 431 ATOM 1656 CA ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1656 CG ILE 431 ATOM 1656 CG ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1656 CG ILE 431 ATOM 1656 CG ILE 431 ATOM 1656 CG ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1656 CG ILE 431 ATOM 1656 CG ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1657 CB ILE 431 ATOM 1656 CG ILE 431 ATOM 1657 CB ILE 431 AT		ATOM	1612 O VAL 425	49.853 16.265 27.269 1.00 15.69	PROT
ATOM 1615 CB THR 426 52.713 18.372 29.667 1.00 12.49 PROT ATOM 1616 OG THR 426 51.890 19.138 30.552 1.00 11.06 PROT ATOM 1618 C THR 426 51.890 19.138 30.552 1.00 11.06 PROT ATOM 1619 O THR 426 52.734 16.928 27.653 1.00 15.72 PROT ATOM 1620 N ASP 427 53.198 17.463 26.651 1.00 14.40 PROT ATOM 1621 CA ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1622 CB ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1623 CG ASP 427 55.874 15.125 29.010 1.00 8.75 PROT ATOM 1625 OD2 ASP 427 55.874 15.125 29.010 1.00 8.75 PROT ATOM 1626 C ASP 427 53.793 14.164 24.856 1.00 25.69 PROT ATOM 1628 N LEU 428 ATOM 1630 CB LEU 428 49.534 13.470 25.00 PROT ATOM 1631 CG LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1632 CD LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1635 CD LEU 428 49.598 1.00 2.00 PROT ATOM 1637 CA ARG 429 ATOM 1636 CB ARG 429 ATOM 1637 CA ARG 429 ATOM 1637 CA ARG 429 ATOM 1640 CD ARG 429 ATOM 1640 CD ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1646 C ARG 4		ATOM	1613 N THR 426	50.753 16.924 29.208 1.00 14.38	PROT
ATOM 1616 OGI THR 426 ATOM 1617 CG2 THR 426 ATOM 1618 C THR 426 ATOM 1619 O THR 426 ATOM 1619 O THR 426 ATOM 1620 N ASP 427 ATOM 1620 CASP 427 ATOM 1621 CA ASP 427 ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 ODI ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1627 O ASP 427 ATOM 1630 CB LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CDI LEU 428 ATOM 1634 C LEU 428 ATOM 1635 O LEU 428 ATOM 1636 CB ASP 427 ATOM 1636 C ASP 427 ATOM 1636 CB LEU 428 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1640 CD ARG 429 ATOM 1640 CD ARG 429 ATOM 1641 NH ARG 429 ATOM 1642 C ARG 429 ATOM 1643 NH ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1646 C ARG 429 ATOM 1647 N MET 430 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1645 C ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1647 N MET 430 ATOM 1648 CA MET 430 ATOM 1649 CB MET 430 ATOM 1650 CG MET 430 ATOM 1651 SD MET 430 ATOM 1655 N ILE 431 ATOM 1656 CA ILE 431 ATOM 1656 CA ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1657 CB ILE 431 ATOM		ATOM	1614 CA THR 426		PROT
ATOM 1618 C THR 426 ATOM 1619 O THR 426 ATOM 1620 N ASP 427 ATOM 1621 CA ASP 427 ATOM 1622 CB ASP 427 ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 OD1 ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1628 N LEU 428 ATOM 1630 CB LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1630 CD LEU 428 ATOM 1630 CD LEU 428 ATOM 1631 CD LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1635 OLE U 428 ATOM 1636 N ARG 429 ATOM 1636 C ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1631 CG ARG 429 ATOM 1634 C LEU 428 ATOM 1635 C ARG 429 ATOM 1636 CA ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1631 CG ARG 429 ATOM 1634 C LEU 428 ATOM 1635 C ARG 429 ATOM 1636 CA ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1631 CG ARG 429 ATOM 1634 C ARG 429 ATOM 1635 C ARG 429 ATOM 1636 CA ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1630 CG ARG 429 ATOM 1630 CB ARG 429 ATOM 1631 CG ARG 429 ATOM 1634 C ARG 429 ATOM 1635 C ARG 429 ATOM 1636 CA ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1639 CG ARG 429 ATOM 1640 NEX ARG 429 ATOM 1640 CD ARG 429 ATOM 1641 NE ARG 429 ATOM 1643 NH1 ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1646 CD ARG 429 ATOM 1647 N MET 430 ATOM 1648 CA MET 430 ATOM 1648 CA MET 430 ATOM 1649 CB MET 430 ATOM 1650 CG MET 430 ATOM 1651 C MET 430 ATOM 1652 CE MET 430 ATOM 1655 N ILE 431 ATOM 1656 CA ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1656 CA ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658	5	ATOM	1615 CB THR 426		PROT
ATOM 1618 C THR 426 52.734 16.928 27.653 1.00 15.72 PROT ATOM 1619 O THR 426 53.198 17.463 26.651 1.00 14.40 PROT ATOM 1620 N ASP 427 53.000 15.672 27.981 1.00 16.23 PROT ATOM 1621 CA ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1622 CB ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1624 OD1 ASP 427 55.377 13.997 29.029 1.00 18.96 PROT ATOM 1624 OD1 ASP 427 55.874 15.125 29.010 1.00 8.75 PROT ATOM 1625 OD2 ASP 427 55.874 15.125 29.010 1.00 8.75 PROT ATOM 1626 C ASP 427 55.579 13.145 29.902 1.00 24.25 PROT ATOM 1627 O ASP 427 53.793 14.164 24.856 1.00 25.69 PROT ATOM 1628 N LEU 428 51.838 14.218 25.986 1.00 5.49 PROT ATOM 1630 CB LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1631 CG LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1632 CD LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1633 CD 2 LEU 428 51.00 8.81 11.00 2.00 PROT ATOM 1634 C LEU 428 51.019 14.987 23.881 1.00 7.72 PROT ATOM 1636 N ARG 429 50.948 17.432 23.659 1.00 7.92 PROT ATOM 1637 CA ARG 429 50.948 17.432 23.659 1.00 7.92 PROT ATOM 1639 CG ARG 429 48.588 19.674 24.935 1.00 10.07 PROT ATOM 1639 CG ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1640 CD ARG 429 48.588 19.674 24.935 1.00 32.08 PROT ATOM 1641 NE ARG 429 45.507 19.955 26.549 1.00 46.8 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 46.8 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 46.08 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 20.00 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 30.24 PROT ATOM 1649 CB MET 430 55.738 17.904 21.737 1.00 28.66 PROT ATOM 1649 CB MET 430 55.738 17.905 24.373 1.00 32.59 PROT ATOM 1651 SD MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1654 O MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1654 O MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1654 O MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1654 O MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1654 O MET 430 55.738 17.905 24.373 1.00 32.52 PROT ATOM 1655 N ILE 431 54.141 14.069 21.196 1.00 15.85 PROT ATOM 1656 CA ILE 431 54.144 14.069 21.196		ATOM	1616 OG1 THR 426	51.890 19.138 30.552 1.00 11.06	PROT
ATOM 1619 O THR 426 53.198 17.463 26.651 1.00 14.40 PROT ATOM 1620 N ASP 427 53.000 15.672 27.981 1.00 16.23 PROT ATOM 1621 CA ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1622 CB ASP 427 55.842 13.630 27.950 1.00 19.48 PROT ATOM 1624 OD1 ASP 427 55.373 13.997 29.029 1.00 18.96 PROT ATOM 1625 OD2 ASP 427 55.579 13.145 29.902 1.00 24.25 PROT ATOM 1626 C ASP 427 53.793 14.164 24.856 1.00 25.69 PROT ATOM 1628 N LEU 428 51.040 13.815 24.849 1.00 2.00 PROT ATOM 1630 CB LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1631 CG LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1632 CD1 LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1634 CD1 LEU 428 51.094 14.987 23.881 1.00 2.00 PROT ATOM 1635 O LEU 428 51.094 14.987 23.881 1.00 2.00 PROT ATOM 1636 N ARG 429 50.948 17.438 23.659 1.00 7.72 PROT ATOM 1638 CB ARG 429 50.948 17.438 23.659 1.00 18.55 PROT ATOM 1639 CG ARG 429 48.588 19.674 24.935 1.00 2.00 PROT ATOM 1641 NE ARG 429 45.860 19.163 24.459 1.00 2.00 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1644 NE ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1646 CA ARG 429 45.860 19.163 24.459 1.00 24.66 PROT ATOM 1646 CA ARG 429 45.860 19.163 24.459		ATOM	1617 CG2 THR 426	53.763 19.283 29.015 1.00 2.93	PROT
ATOM 1620 N ASP 427 53.000 15.672 27.981 1.00 16.23 PROT ATOM 1621 CA ASP 427 53.865 14.843 27.157 1.00 16.35 PROT ATOM 1623 CG ASP 427 55.337 13.997 29.029 1.00 18.96 PROT ATOM 1625 OD2 ASP 427 55.874 15.125 29.010 1.00 8.75 PROT ATOM 1626 C ASP 427 55.579 13.145 29.902 1.00 24.25 PROT ATOM 1626 C ASP 427 53.155 14.381 25.891 1.00 20.52 PROT ATOM 1628 N LEU 428 51.838 14.218 25.986 1.00 25.69 PROT ATOM 1629 CA LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1630 CB LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1631 CG LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1633 CD2 LEU 428 48.184 11.789 26.481 1.00 2.00 PROT ATOM 1635 C D LEU 428 51.092 14.800 22.666 1.00 9.22 78.004 16.340 16.3		ATOM	1618 C THR 426		PROT
ATOM 1621 CA ASP 427 ATOM 1622 CB ASP 427 ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 OD1 ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1628 N LEU 428 ATOM 1630 CB LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1631 CG LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1634 C LEU 428 ATOM 1635 O LEU 428 ATOM 1635 O LEU 428 ATOM 1636 N ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1640 CD ARG 429 ATOM 1650 CG MET 430 ATOM 1654 C ARG 429 ATOM 1655 N ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431 ATOM 1658		ATOM	1619 O THR 426		PROT
ATOM 1622 CB ASP 427 ATOM 1623 CG ASP 427 ATOM 1624 OD1 ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1625 OD2 ASP 427 ATOM 1626 C ASP 427 ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1628 N LEU 428 ATOM 1629 CA LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1635 O LEU 428 ATOM 1636 N ARG 429 ATOM 1636 N ARG 429 ATOM 1636 CB ARG 429 ATOM 1637 CA ARG 429 ATOM 1639 CG ARG 429 ATOM 1640 CD ARG 429 ATOM 1640 CD ARG 429 ATOM 1641 NE ARG 429 ATOM 1643 NH1 ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1646 C ARG 429 ATOM 1646 C ARG 429 ATOM 1647 N MET 430 ATOM 1650 CG MET 430 ATOM 1651 SD MET 430 ATOM 1654 O MET 430 ATOM 1655 N ILE 431 ATOM 1655 CG ILE 431 ATOM 1656 CA ILE 431 ATOM 1656 CA ILE 431 ATOM 1657 CB ILE 431 ATOM 1658 CG2 ILE 431	10	ATOM	1620 N ASP 427	53.000 15.672 27.981 1.00 16.23	PROT
ATOM 1623 CG ASP 427		ATOM	1621 CA ASP 427		PROT
ATOM 1624 OD1 ASP 427 S5.874 15.125 29.010 1.00 8.75 PROT ATOM 1625 OD2 ASP 427 S5.579 13.145 29.902 1.00 24.25 PROT ATOM 1626 C ASP 427 S3.155 14.381 25.891 1.00 20.52 PROT ATOM 1628 N LEU 428 S1.838 14.218 25.986 1.00 25.69 PROT ATOM 1630 CB LEU 428 S1.838 14.218 25.986 1.00 25.69 PROT ATOM 1630 CB LEU 428 S1.040 13.815 24.849 1.00 2.00 PROT ATOM 1631 CG LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1632 CD1 LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1633 CD2 LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1636 N ARG 429 S0.088 11.080 25.108 1.00 2.00 PROT ATOM 1636 N ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1636 N ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1630 CD ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1640 CD ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1640 CD ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1640 CD ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1644 NH2 ARG 429 47.508 19.923 25.880 1.00 42.46 PROT ATOM 1644 NH2 ARG 429 45.807 19.63 24.459 1.00 33.35 PROT ATOM 1644 NH2 ARG 429 45.807 19.65 24.459 1.00 30.34 PROT ATOM 1646 C ARG 429 45.307 19.955 26.549 1.00 46.08 PROT ATOM 1648 C AMET 430 55.738 17.015 24.100 1.00 30.24 PROT ATOM 1650 CG MET 430 55.727 19.795 24.373 1.00 35.91 PROT ATOM 1654 C MET 430 55.727 19.795 24.373 1.00 35.91 PROT ATOM 1655 C MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 C MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 C MET 430 55.287 16.560 20.860		ATOM	1622 CB ASP 427	54.342 13.630 27.950 1.00 19.48	
ATOM 1625 OD2 ASP 427 S5.579 13.145 29.902 1.00 24.25 PROT ATOM 1626 C ASP 427 S3.155 14.381 25.891 1.00 25.69 PROT ATOM 1628 N LEU 428 S1.838 14.218 25.986 1.00 5.49 PROT ATOM 1629 CA LEU 428 S1.838 14.218 25.986 1.00 5.49 PROT ATOM 1630 CB LEU 428 49.634 13.470 25.301 1.00 2.00 PROT ATOM 1631 CG LEU 428 49.579 12.127 26.028 1.00 2.00 PROT ATOM 1632 CD1 LEU 428 48.184 11.789 26.481 1.00 2.00 PROT ATOM 1633 CD2 LEU 428 51.091 14.987 23.881 1.00 7.72 PROT ATOM 1636 N ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1636 N ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1636 CA ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1630 CB ARG 429 S0.961 16.197 24.432 1.00 10.07 PROT ATOM 1630 CG ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1640 CD ARG 429 49.548 18.634 25.429 1.00 14.80 PROT ATOM 1640 CD ARG 429 47.508 19.923 25.880 1.00 22.60 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 46.08 PROT ATOM 1644 NH2 ARG 429 45.307 19.955 26.549 1.00 46.08 PROT ATOM 1646 C ARG 429 52.298 17.904 21.737 1.00 28.66 PROT ATOM 1649 CB MET 430 53.434 17.270 23.629 1.00 20.26 PROT ATOM 1649 CB MET 430 55.738 17.015 24.100 1.00 30.21 PROT ATOM 1651 CG MET 430 55.727 19.795 24.373 1.00 35.91 PROT ATOM 1654 C MET 430 55.727 19.795 24.373 1.00 35.91 PROT ATOM 1655 N MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 N MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 N MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 N LE 431 54.144 14.069 21.795		ATOM	1623 CG ASP 427		PROT
ATOM 1626 C ASP 427 ATOM 1627 O ASP 427 ATOM 1627 O ASP 427 ATOM 1628 N LEU 428 ATOM 1629 CA LEU 428 ATOM 1630 CB LEU 428 ATOM 1630 CB LEU 428 ATOM 1631 CG LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1632 CD1 LEU 428 ATOM 1633 CD2 LEU 428 ATOM 1634 C LEU 428 ATOM 1635 O LEU 428 ATOM 1636 N ARG 429 ATOM 1636 N ARG 429 ATOM 1637 CA ARG 429 ATOM 1638 CB ARG 429 ATOM 1639 CG ARG 429 ATOM 1640 CD ARG 429 ATOM 1640 CD ARG 429 ATOM 1641 NE ARG 429 ATOM 1644 NH2 ARG 429 ATOM 1645 C ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1646 O ARG 429 ATOM 1646 CD ARG 429 ATOM 1646 CD ARG 429 ATOM 1647 N MET 430 ATOM 1648 CA MET 430 ATOM 1649 CB MET 430 ATOM 1655 CG MET 430 ATOM 1655 CG MET 430 ATOM 1655 CG ILE 431 ATOM 1655 CG ILE 431 ATOM 1655 CG ILE 431 ATOM 1657 CB ILE 431 S5.727 12.084 20.539 1.00 11.11 PROT		ATOM	1624 OD1 ASP 427		
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ATOM 1630 CB LEU 428		ATOM	1628 N LEU 428	51.838 14.218 25.986 1.00 5.49	PROT
ATOM 1631 CG LEU 428		ATOM	1629 CA LEU 428	51.040 13.815 24.849 1.00 2.00	PROT
ATOM 1632 CD1 LEU 428	20	ATOM	1630 CB LEU 428	49.634 13.470 25.301 1.00 2.00	PROT
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40 ATOM 1650 CG MET 430 56.061 18.165 25.056 1.00 34.66 PROT ATOM 1651 SD MET 430 55.727 19.795 24.373 1.00 35.91 PROT ATOM 1652 CE MET 430 56.839 19.814 22.978 1.00 32.52 PROT ATOM 1653 C MET 430 54.735 16.302 21.925 1.00 18.70 PROT ATOM 1654 O MET 430 55.287 16.560 20.860 1.00 16.59 PROT ATOM 1655 N ILE 431 54.161 15.133 22.182 1.00 15.38 PROT ATOM 1656 CA ILE 431 54.144 14.069 21.196 1.00 15.85 PROT ATOM 1658 CG2 ILE 431 52.727 12.084 20.539 1.00 11.11 PROT					
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ATOM 1659 CG1 ILE 431 54.239 11.924 22.489 1.00 11.72 PROT					
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50 ATOM 1660 CD1 ILE 431 53.552 11.224 23.615 1.00 16.22 PROT	50	ATOM	1660 CD1 ILE 431	53.552 11.224 23.615 1.00 16.22	PKOT

	ATOM	1661 C ILE 431 53.	.538 14.609 19.904 1.00 18.49	PROT
	ATOM		.134 14.483 18.839 1.00 17.36	PROT
	ATOM		2.361 15.220 20.003 1.00 2.00	PROT
	ATOM		51.721 15.772 18.831 1.00 2.00	PROT
5	ATOM		2.542 16.851 18.148 1.00 10.55	PROT
,	ATOM		2.707 16.834 16.936 1.00 9.60	PROT
	ATOM		3.043 17.805 18.926 1.00 11.17	PROT
	ATOM		53.855 18.884 18.385 1.00 2.00	PROT
	ATOM		54.326 19.771 19.506 1.00 2.00	PROT
10	ATOM		5.050 18.285 17.646 1.00 6.43	PROT
10	ATOM		5.493 18.789 16.623 1.00 11.71	PROT
	ATOM		5.579 17.197 18.179 1.00 15.71	PROT
	ATOM		56.715 16.534 17.573 1.00 13.44	PROT
	ATOM		57.228 15.464 18.518 1.00 14.76	PROT
15	ATOM		88.910 15.703 18.985 1.00 20.82	PROT
15	ATOM		5.269 15.902 16.264 1.00 9.28	PROT
	ATOM		6.969 15.948 15.256 1.00 8.50	PROT
	ATOM		.091 15.300 16.298 1.00 11.04	PROT
	ATOM		4.533 14.657 15.122 1.00 11.30	PROT
20	ATOM		3.142 14.132 15.438 1.00 4.30	PROT
20	ATOM		2.480 13.460 14.283 1.00 13.68	PROT
	ATOM		52.751 12.288 13.662 1.00 4.72	PROT
	ATOM		51.358 13.976 13.666 1.00 5.53	PROT
	ATOM		0.966 13.147 12.717 1.00 12.84	PROT
25	ATOM	1685 NE2 HIS 435	51.794 12.116 12.694 1.00 15.77	PROT
	ATOM		.482 15.661 13.973 1.00 8.50	PROT
	ATOM		.941 15.370 12.869 1.00 14.82	PROT
	ATOM		3.938 16.844 14.245 1.00 5.74	PROT
	ATOM		53.843 17.905 13.252 1.00 2.00	PROT
30	ATOM	1690 CB ALA 436	53.632 19.241 13.942 1.00 2.00	PROT
	ATOM	1691 C ALA 436 5	5.121 17.934 12.406 1.00 8.68	PROT
	ATOM		5.080 17.712 11.193 1.00 15.14	PROT
	ATOM	1693 N SER 437 56	5.256 18.189 13.047 1.00 6.82	PROT
	ATOM		57.522 18.226 12.337 1.00 9.05	PROT
35	ATOM		88.671 18.511 13.295 1.00 2.00	PROT
	ATOM		59.593 19.406 12.699 1.00 21.18	PROT
	ATOM		7.758 16.896 11.637 1.00 15.18	PROT
	ATOM		8.076 16.849 10.445 1.00 19.33	PROT
	ATOM	1699 N ARG 438 5	7.607 15.805 12.373 1.00 16.98	PROT
40	ATOM		57.799 14.501 11.766 1.00 16.98	PROT
	ATOM		57.294 13.409 12.702 1.00 24.77	PROT
	ATOM		58.006 12.086 12.534 1.00 33.76	
	ATOM		59.506 12.280 12.614 1.00 30.64	PROT
	ATOM		60.219 11.380 11.721 1.00 29.76	PROT
45	ATOM	1705 CZ ARG 438	61.505 11.504 11.423 1.00 25.21	PROT
	ATOM		62.077 10.641 10.603 1.00 39.58	
	ATOM		62.217 12.492 11.942 1.00 14.13	
	ATOM		7.031 14.441 10.448 1.00 16.49	PROT
	ATOM ATOM		57.563 14.008 9.424 1.00 15.57 5.781 14.893 10.484 1.00 16.75	PROT PROT

	4 TO 1 (1711 CA DITE 420	54.933 14.878 9.303 1.00 21.63	PROT
	ATOM	1711 CA PHE 439	53.603 15.575 9.574 1.00 17.84	PROT
	ATOM ATOM	1712 CB PHE 439 1713 CG PHE 439	52.597 15.364 8.490 1.00 20.60	PROT
			52.042 14.103 8.279 1.00 30.60	PROT
_	ATOM	1714 CD1 PHE 439	52.265 16.394 7.622 1.00 14.95	PROT
5	ATOM	1715 CD2 PHE 439	51.175 13.867 7.206 1.00 29.12	PROT
	ATOM	1716 CE1 PHE 439		PROT
	ATOM	1717 CE2 PHE 439		PROT
	ATOM	1718 CZ PHE 439		PROT
10	ATOM	1719 C PHE 439		PROT
10	ATOM	1720 O PHE 439 1721 N LEU 440		
	ATOM		56.328 16.633 8.427 1.00 26.77	PROT
	ATOM	1722 CA LEU 440	57.055 17.382 7.418 1.00 24.66	PROT
	ATOM	1723 CB LEU 440	57.555 18.696 8.005 1.00 10.80	PROT
	ATOM	1724 CG LEU 440	56.501 19.658 8.541 1.00 8.60	PROT
15	ATOM	1725 CD1 LEU 440	57.152 20.985 8.855 1.00 17.69	PROT
	ATOM	1726 CD2 LEU 440	55.410 19.847 7.522 1.00 15.71	PROT
	ATOM	1727 C LEU 440	58.245 16.578 6.912 1.00 29.61	PROT
	ATOM	1728 O LEU 440	58.506 16.526 5.718 1.00 32.37	PROT
	ATOM	1729 N HIS 441	58.971 15.954 7.830 1.00 28.12	PROT
20	ATOM	1730 CA HIS 441	60.140 15.172 7.460 1.00 28.51	PROT
	ATOM	1731 CB HIS 441	60.783 14.564 8.705 1.00 36.77	PROT
	ATOM	1732 C HIS 441	59.724 14.081 6.497 1.00 31.94	PROT
	ATOM	1733 O HIS 441	60.461 13.725 5.579 1.00 49.29	PROT
25	ATOM	1734 N MET 442	58.533 13.545 6.711 1.00 41.16	PROT
25	ATOM	1735 CA MET 442	58.033 12.487 5.854 1.00 39.99	PROT
	ATOM	1736 CB MET 442	56.871 11.776 6.551 1.00 38.32	PROT
	ATOM	1737 CG MET 442	57.263 11.122 7.860 1.00 19.20	PROT
	ATOM	1738 SD MET 442	55.859 10.350 8.675 1.00 38.06	PROT
20	ATOM	1739 CE MET 442	54.906 11.767 9.073 1.00 21.45	PROT
30	ATOM	1740 C MET 442	57.599 13.031 4.495 1.00 35.68	PROT
	ATOM	1741 O MET 442	57.887 12.431 3.461 1.00 27.43	PROT
	ATOM	1742 N LYS 443	56.920 14.175 4.503 1.00 34.17	PROT
	ATOM	1743 CA LYS 443	56.447 14.796 3.268 1.00 34.33	PROT
	ATOM	1744 CB LYS 443	55.767 16.129 3.574 1.00 21.68	PROT
35	ATOM	1745 CG LYS 443	54.303 15.989 3.953 1.00 26.95	PROT
	ATOM	1746 CD LYS 443	53.497 17.231 3.602 1.00 30.78	PROT
	ATOM	1747 CE LYS 443	52.204 16.848 2.861 1.00 56.06	PROT
	ATOM	1748 NZ LYS 443	50.931 17.261 3.564 1.00 45.26	PROT
40	ATOM	1749 C LYS 443	57.570 15.007 2.251 1.00 37.81	PROT
40	ATOM	1750 O LYS 443	57.325 15.049 1.041 1.00 38.26	PROT
	ATOM	1751 N VAL 444	58.798 15.130 2.741 1.00 25.12	PROT
	ATOM	1752 CA VAL 444	59.942 15.318 1.867 1.00 25.43	PROT
	ATOM	1753 CB VAL 444	60.802 16.531 2.334 1.00 29.15	PROT
	ATOM	1754 CG1 VAL 444	59.893 17.621 2.861 1.00 29.48	PROT
45	ATOM	1755 CG2 VAL 444	61.785 16.121 3.419 1.00 36.65	PROT
	ATOM	1756 C VAL 444	60.786 14.042 1.825 1.00 30.03	PROT
	ATOM	1757 O VAL 444	62.009 14.099 1.698 1.00 39.43	PROT
	ATOM	1758 N GLU 445	60.127 12.888 1.903 1.00 39.84	PROT
	ATOM	1759 CA GLU 445	60.842 11.612 1.896 1.00 43.07	PROT
50	ATOM	1760 CB GLU 445	61.429 11.360 3.282 1.00 50.55	PROT

	ATOM	1761 CG GLU 445	62.399 10.203 3.351 1.00 77.00	PROT
	ATOM	1762 CD GLU 445	63.569 10.495 4.267 1.00 98.21	PROT
	ATOM	1763 OE1 GLU 445	64.251 9.538 4.701 1.00100.00	PROT
	ATOM	1764 OE2 GLU 445	63.804 11.690 4.554 1.00100.00	
5	ATOM	1765 C GLU 445	59.989 10.408 1.491 1.00 43.41	PROT
	ATOM	1766 O GLU 445	60.466 9.274 1.511 1.00 48.80	PROT
	ATOM	1767 N CYS 446	58.731 10.644 1.137 1.00 38.17	PROT
	ATOM	1768 CA CYS 446	57.852 9.548 0.743 1.00 41.38	PROT
	ATOM	1769 CB CYS 446	57.066 9.035 1.965 1.00 40.61	PROT
10	ATOM	1770 SG CYS 446	58.062 8.276 3.320 1.00 44.73	PROT
	ATOM	1771 C CYS 446	56.886 10.003 -0.362 1.00 45.83	PROT
	ATOM	1772 O CYS 446	56.466 11.184 -0.323 1.00 44.17	PROT
	ATOM	1773 OT CYS 446	56.570 9.180 -1.259 1.00 40.79	PROT
	ATOM	1774 CB GLU 449	52.635 12.140 -2.649 1.00 28.60	PROT
15	ATOM	1775 C GLU 449	52.019 10.014 -1.526 1.00 38.06	PROT
	ATOM	1776 O GLU 449	50.873 10.220 -1.935 1.00 43.52	PROT
	ATOM	1777 N GLU 449	54.378 10.460 -2.167 1.00 17.78	PROT
	ATOM	1778 CA GLU 449	53.105 11.069 -1.689 1.00 33.80	PROT
	ATOM	1779 N LEU 450	52.387 8.880 -0.936 1.00 46.88	PROT
20	ATOM	1780 CA LEU 450	51.432 7.808 -0.696 1.00 52.62	PROT
	ATOM	1781 CB LEU 450	52.101 6.436 -0.850 1.00 57.50	PROT
	ATOM	1782 CG LEU 450	53.338 6.066 -0.028 1.00 59.81	PROT
	ATOM	1783 CD1 LEU 450	53.613 4.573 -0.198 1.00 51.33	PROT
	ATOM	1784 CD2 LEU 450	54.544 6.890 -0.473 1.00 57.03	PROT
25	ATOM	1785 C LEU 450	50.850 7.970 0.711 1.00 50.65	PROT
	ATOM	1786 O LEU 450	50.965 7.091 1.569 1.00 38.49	PROT
	ATOM	1787 N PHE 451	50.225 9.123 0.923 1.00 32.24	PROT
	ATOM	1788 CA PHE 451	49.602 9.478 2.188 1.00 32.64	PROT
	ATOM	1789 CB PHE 451	50.091 10.857 2.648 1.00 56.06	PROT
30	ATOM	1790 CG PHE 451	51.534 10.895 3.056 1.00 61.73	PROT
	ATOM	1791 CD1 PHE 451	52.523 10.366 2.235 1.00 66.92	PROT
	ATOM	1792 CD2 PHE 451	51.905 11.486 4.256 1.00 58.76	PROT
	ATOM	1793 CE1 PHE 451	53.860 10.430 2.604 1.00 69.17	PROT
	ATOM	1794 CE2 PHE 451	53.231 11.556 4.635 1.00 61.48	PROT
35	ATOM	1795 CZ PHE 451	54.214 11.028 3.809 1.00 71.95	PROT
	ATOM	1796 C PHE 451	48.081 9.548 2.025 1.00 30.67	PROT
	ATOM	1797 O PHE 451	47.571 10.429 1.324 1.00 38.49	PROT
	ATOM	1798 N PRO 452	47.336 8.627 2.672 1.00 19.14	PROT
40	ATOM	1799 CD PRO 452	47.774 7.495 3.510 1.00 24.21	PROT
40	ATOM	1800 CA PRO 452	45.881 8.672 2.538 1.00 5.88	PROT
	ATOM	1801 CB PRO 452	45.397 7.742 3.633 1.00 16.92	PROT
	ATOM	1802 CG PRO 452	46.496 6.737 3.761 1.00 16.91	PROT
	ATOM	1803 C PRO 452	45.354 10.090 2.687 1.00 15.15	PROT
15	ATOM	1804 O PRO 452	45.879 10.886 3.463 1.00 22.59	PROT
45	ATOM	1805 N PRO 453	44.315 10.429 1.920 1.00 18.37	PROT
	ATOM	1806 CD PRO 453	43.653 9.540 0.951 1.00 3.83	PROT
	ATOM	1807 CA PRO 453	43.710 11.766 1.960 1.00 14.00 42.502 11.649 1.032 1.00 20.04	PROT
	ATOM	1808 CB PRO 453 1809 CG PRO 453	42.316 10.163 0.807 1.00 20.04	PROT
50	ATOM ATOM	1810 C PRO 453	43.321 12.277 3.346 1.00 14.70	PROT PROT
<i>5</i> 0	A I OM	1010 C FKO 422	1.00 14.70	INOI

	ATOM	1811 O PRO 453	43.609 13.422 3.682 1.00 9.70	PROT
	ATOM	1812 N LEU 454	42.667 11.446 4.152 1.00 25.39	PROT
	ATOM	1813 CA LEU 454	42.261 11.886 5.491 1.00 28.61	PROT
	ATOM	1814 CB LEU 454	41,463 10.804 6.217 1.00 17.29	PROT
5	ATOM	1815 CG LEU 454	40.893 11.224 7.572 1.00 9.05	PROT
	ATOM	1816 CD1 LEU 454	40.174 12.547 7.435 1.00 17.23	PROT
	ATOM	1817 CD2 LEU 454	39.946 10.148 8.079 1.00 8.05	PROT
	ATOM	1818 C LEU 454	43.479 12.234 6.316 1.00 23.36	PROT
	ATOM	1819 O LEU 454	43.484 13.225 7.037 1.00 10.99	PROT
10	ATOM	1820 N PHE 455	44.503 11.394 6.205 1.00 14.26	PROT
	ATOM	1821 CA PHE 455	45.769 11.595 6.902 1.00 15.33	PROT
	ATOM	1822 CB PHE 455	46.761 10.496 6.501 1.00 26.32	PROT
	ATOM	1823 CG PHE 455	48.138 10.644 7.108 1.00 43.03	PROT
	ATOM	1824 CD1 PHE 455	48.305 11.094 8.414 1.00 43.52	PROT
15	ATOM	1825 CD2 PHE 455	49.270 10.282 6.380 1.00 41.44	PROT
13	ATOM	1826 CE1 PHE 455	49.576 11.176 8.987 1.00 37.77	PROT
	ATOM	1827 CE2 PHE 455	50.536 10.363 6.947 1.00 49.43	PROT
	ATOM	1828 CZ PHE 455	50.686 10.811 8.255 1.00 39.99	PROT
	ATOM	1829 C PHE 455	46.313 12.956 6.500 1.00 19.37	PROT
20	ATOM	1830 O PHE 455	46.945 13.646 7.298 1.00 29.31	PROT
	ATOM	1831 N LEU 456	46.048 13.345 5.257 1.00 17.16	PROT
	ATOM	1832 CA LEU 456	46.527 14.625 4.750 1.00 20.15	PROT
	ATOM	1833 CB LEU 456	46.572 14.603 3.218 1.00 35.14	PROT
	ATOM	1834 CG LEU 456	47.593 13.660 2.568 1.00 40.45	PROT
25	ATOM	1835 CD1 LEU 456	47.233 13.456 1.116 1.00 44.38	PROT
	ATOM	1836 CD2 LEU 456	48.990 14.234 2.680 1.00 34.88	PROT
	ATOM	1837 C LEU 456	45.680 15.800 5.226 1.00 20.37	PROT
	ATOM	1838 O LEU 456	46.207 16.866 5.548 1.00 29.61	PROT
	ATOM	1839 N GLU 457	44.367 15.607 5.280 1.00 13.06	PROT
30	ATOM	1840 CA GLU 457	43.483 16.675 5.713 1.00 14.14	PROT
	ATOM	1841 CB GLU 457	42.037 16.256 5.516 1.00 29.57	PROT
	ATOM	1842 C GLU 457	43.731 17.058 7.173 1.00 14.95	PROT
	ATOM	1843 O GLU 457	43.771 18.237 7.514 1.00 15.98	PROT
	ATOM	1844 N VAL 458	43.901 16.051 8.026 1.00 26.34	PROT
35	ATOM	1845 CA VAL 458	44.143 16.260 9.455 1.00 24.39	PROT
	ATOM	1846 CB VAL 458	44.219 14.910 10.208 1.00 20.14	PROT
	ATOM	1847 CG1 VAL 458	44.882 15.102 11.554 1.00 22.01	PROT
	ATOM	1848 CG2 VAL 458	42.831 14.341 10.400 1.00 28.11	PROT
	ATOM	1849 C VAL 458	45,417 17.039 9.778 1.00 21.50	PROT
40	ATOM	1850 O VAL 458	45.364 18.062 10.439 1.00 18.85	PROT
_	ATOM	1851 N PHE 459	46.557 16.546 9.308 1.00 16.05	PROT
	ATOM	1852 CA PHE 459	47.840 17.174 9.586 1.00 20.28	PROT
	ATOM	1853 CB PHE 459	48.862 16.072 9.846 1.00 20.26	PROT
	ATOM	1854 CG PHE 459	48.389 15.055 10.833 1.00 27.22	PROT
45	ATOM	1855 CD1 PHE 459	47.917 13.822 10.408 1.00 28.01	PROT
	ATOM	1856 CD2 PHE 459	48.390 15.339 12.204 1.00 40.66	PROT
	ATOM	1857 CE1 PHE 459	47.447 12.876 11.334 1.00 21.78	PROT
	ATOM	1858 CE2 PHE 459	47.922 14.402 13.140 1.00 25.98	PROT
	ATOM	1859 CZ PHE 459	47.450 13.172 12.702 1.00 17.63	PROT
50	ATOM	1860 C PHE 459	48.381 18.152 8.540 1.00 23.03	PROT

	ATOM	1861 O PHE 459 4	9.601 18.311 8.416 1.00 27.34	PROT
	ATOM	1862 N GLU 460 4	47.480 18.816 7.815 1.00 33.88	PROT
	ATOM	1863 CA GLU 460	47.846 19.774 6.767 1.00 36.60	PROT
	ATOM	1864 CB GLU 460	48.930 20.732 7.257 1.00 46.04	PROT
5	ATOM	1865 CG GLU 460	48.406 21.899 8.054 1.00 67.27	PROT
	ATOM	1866 CD GLU 460	47.298 22.636 7.339 1.00 71.34	PROT
	ATOM	1867 OE1 GLU 460	47.448 23.859 7.121 1.00 71.99	PROT
	ATOM	1868 OE2 GLU 460	46.280 21.993 6.998 1.00 72.73	PROT
	ATOM	1869 C GLU 460 4	18.353 19.037 5.535 1.00 46.31	PROT
10	ATOM	1870 O GLU 460	48.642 17.829 5.655 1.00 51.79	PROT
	ATOM	1871 OT GLU 460	48.461 19.669 4.462 1.00 60.92	PROT
	ATOM	1872 C1 GC1 1 47	7.011 4.539 15.912 1.00 29.38	LIGA
	ATOM	1873 C2 GC1 1 5	1.292 6.537 13.571 1.00 17.11	LIGA
	ATOM	1874 C3 GC1 1 4	7.393 4.205 14.573 1.00 33.72	LIGA
15	ATOM	1875 C4 GC1 1 52	2.119 6.409 12.400 1.00 19.76	LIGA
	ATOM	1876 C5 GC1 1 48	8.689 4.481 14.089 1.00 25.02	LIGA
	ATOM	1877 C6 GC1 1 52	2.344 7.525 11.539 1.00 17.51	LIGA
	ATOM		9.684 5.122 14.949 1.00 23.99	LIGA
	ATOM		1.722 8.778 11.873 1.00 20.21	LIGA
20	ATOM		9.283 5.452 16.318 1.00 18.19	LIGA
	ATOM	1881 C10 GC1 1 5	0.906 8.928 13.018 1.00 15.43	LIGA
	ATOM		7.973 5.163 16.779 1.00 30.64	LIGA
	ATOM		0.696 7.827 13.850 1.00 25.06	LIGA
	ATOM		5.700 4.254 16.325 1.00 28.60	LIGA
25	ATOM		33.198 7.459 10.291 1.00 20.30	LIGA
	ATOM		5.305 3.866 17.666 1.00 18.51	LIGA
	ATOM		52.423 6.824 9.131 1.00 17.21	LIGA
	ATOM		3.816 4.078 17.872 1.00 21.43	LIGA
	ATOM	-	4.514 6.689 10.543 1.00 24.97	LIGA
30	ATOM		8.994 4.093 12.664 1.00 33.46	LIGA
	ATOM		50.243 6.110 17.278 1.00 27.69	LIGA
	ATOM		1.902 9.861 11.086 1.00 23.34	LIGA
	ATOM	,,	51.026 5.430 14.458 1.00 22.49	LIGA
	ATOM		3.147 3.117 18.247 1.00 18.06	LIGA
35	ATOM	1895 O4 GC1 1 4	3.331 5.204 17.665 1.00 28.27	LIGA
	END			

PCT/US98/25296 WO 99/26966

APPENDIX 8

TRBGC1.PDB

REMARK TR-beta GC-2 Full length numbering

REMARK refinement resolution: 100.00 - 2.40 A starting r= 0.2602 free r= 0.2960

final r = 0.2532 free_r = 0.2894REMARK

REMARK sg= P3(1)21 a= 68.9 b= 68.9 c= 131.5 alpha= 90 beta= 90 gamma= 120

REMARK theoretical total number of refl. in resol. range: 14710 (100.0 %)

REMARK number of unobserved reflections (no entry or |F|=0): 336 (2.3 %)

REMARK number of reflections rejected:

0(0.0%)

10 REMARK total number of reflections used: 14374 (97.7 %)

REMARK number of reflections in working set:

13656 (92.8%)

REMARK number of reflections in test set:

718 (4.9 %)

REMARK

REMARK ALA 199 to ALA 201 from His-tag

15 REMARK

REMARK Four cacodylate-modified cysteines (CYA)

REMARK Cys294, Cys298, Cys388, Cys434

REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density; 20

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK amino acid sequence confirmed,

REMARK differing from that reported by Weinberger et. al.

25 REMARK in the following codons:

REMARK 243 Pro - Arg

REMARK 337 lle - Thr

REMARK 451 Leu - Phe

REMARK as reported by Sakurai et. al.

30 REMARK note also correction of initiation codon,

REMARK yielding a polypeptide of 461 amino acids

JRNL AUTH A.SAKURAI, A.NAKAI, L.J. DEGROOT

JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE RECEPTOR

35 JRNL TITL2 BETA GENE

> JRNL REF MOL.CELL.ENDO. V.71 1990

JRNL AUTH

C.WEINBERGER,

C.C.THOMPSON,R.LEBO,D.J.GRUOL,R.M.EVANS

JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE

40 RECEPTOR

> JRNL REF **NATURE**

V.324 6098 1986

ATOM 1 CB ALA 199 36.564 26.104 43.169 1.00 73.87

34.723 26.996 44.613 1.00 78.22 ATOM 2 C ALA 199

3 O ALA 199 34.741 28.230 44.568 1.00 81.84 ATOM

45 4 N ALA 199 34.389 26.744 42.166 1.00 77.76 ATOM

5 CA ALA 199 35.048 26.165 43.375 1.00 77.98 ATOM

6 N ALA 200 34.428 26.309 45.713 1.00 77.78 ATOM

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34.098 26.961 46.984 1.00 77.03
             7 CA ALA 200
    ATOM
                               32.761 27.693 46.865 1.00 79.04
             8 CB ALA 200
    ATOM
                              34.028 25.897 48.084 1.00 75.79
              9 C ALA 200
    ATOM
             10 O ALA 200
                               34.877 25.857 48.978 1.00 71.58
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             11 N ALA 201
                               33.005 25.050 48.010 1.00 73.70
    ATOM
                               32.838 23.968 48.972 1.00 70.15
             12 CA ALA 201
    ATOM
                               31.468 23.328 48.809 1.00 71.16
             13 CB ALA 201
    ATOM
                              33.934 22.963 48.642 1.00 67.54
             14 C ALA 201
    ATOM
                               34.218 22.044 49.413 1.00 67.14
             15 O ALA 201
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             16 N GLU 202
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    ATOM
                               35.624 22.325 46.975 1.00 59.45
             17 CA GLU 202
    ATOM
                               35.835 22.621 45.482 1.00 55.12
             18 CB GLU 202
    ATOM
                                36.820 21.716 44.749 1.00 56.25
             19 CG GLU 202
    ATOM
                                36.382 20.260 44.723 1.00 54.99
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             21 OE1 GLU 202
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15
                                37.210 19.385 45.050 1.00 59.90
             22 OE2 GLU 202
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             23 C GLU 202
                               36.885 22.674 47.770 1.00 55.96
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                               37.472 21.823 48.435 1.00 52.90
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             24 O GLU 202
                               37.282 23.943 47.698 1.00 54.95
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             25 N GLU 203
     ATOM
             26 CA GLU 203
                               38.464 24.434 48.390 1.00 55.59
20
             27 CB GLU 203
                               38.632 25.924 48.126 1.00 53.21
     ATOM
             28 C GLU 203
                               38.415 24.171 49.894 1.00 56.30
     ATOM
             29 O GLU 203
                               39.445 23.948 50.526 1.00 58.70
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             30 N LEU 204
                               37.213 24.193 50.462 1.00 57.14
     ATOM
             31 CA LEU 204
                               37.038 23.966 51.893 1.00 56.93
     ATOM
25
                               35.658 24.465 52.338 1.00 58.31
             32 CB LEU 204
     ATOM
             33 CG LEU 204
                               35.348 24.508 53.839 1.00 51.69
     ATOM
                                36.314 25.446 54.549 1.00 44.38
             34 CD1 LEU 204
     ATOM
             35 CD2 LEU 204
                                33.920 24.986 54.039 1.00 52.44
     ATOM
                               37.198 22.489 52.246 1.00 58.20
     ATOM
             36 C LEU 204
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     ATOM
             37 O LEU 204
                               37.831 22.155 53.252 1.00 58.99
                               36.620 21.607 51.431 1.00 58.26
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     ATOM
                                36.736 20.167 51.657 1.00 55.38
             39 CA GLN 205
     ATOM
             40 CB GLN 205
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                                34.498 19.324 50.741 1.00 53.33
             41 CG GLN 205
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     ATOM
             42 CD GLN 205
                                33.854 18.520 49.629 1.00 53.40
     ATOM
                                33.850 18.939 48.473 1.00 51.68
             43 OE1 GLN 205
     ATOM
                                33.325 17.352 49.968 1.00 51.34
             44 NE2 GLN 205
     ATOM
                               38.200 19.775 51.608 1.00 55.05
             45 C GLN 205
     ATOM
                               38.665 18.964 52.407 1.00 53.63
     ATOM
             46 O GLN 205
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             47 N LYS 206
                               38.918 20.348 50.648 1.00 53.55
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             48 CA LYS 206
                                40.337 20.078 50.493 1.00 57.40
     ATOM
                               40.896 20.814 49.269 1.00 58.94
             49 CB LYS 206
     ATOM
              50 CG LYS 206
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     ATOM
                                40.921 21.141 46.781 1.00 72.50
              51 CD LYS 206
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     ATOM
                               40.346 20.695 45.445 1.00 75.60
     ATOM
              52 CE LYS 206
                               40.945 21.445 44.304 1.00 77.08
              53 NZ LYS 206
     ATOM
                               41.053 20.559 51.747 1.00 53.98
             54 C LYS 206
     ATOM
                               41.905 19.866 52.300 1.00 53.49
              55 O LYS 206
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             56 N SER 207
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     ATOM
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              57 CA SER 207
                                41.254 22.386 53.364 1.00 51.49
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              58 CB SER 207
                                40.546 23.715 53.619 1.00 51.01
              59 OG SER 207
                                41.108 24.383 54.731 1.00 63.00
     ATOM
              60 C SER 207
                               41.178 21.502 54.616 1.00 49.49
     ATOM
              61 O SER 207
                               42.073 21.538 55.465 1.00 47.44
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              62 N ILE 208
                               40.117 20.707 54.725 1.00 44.39
     ATOM
              63 CA ILE 208
                               39.938 19.829 55.874 1.00 45.99
     ATOM
     ATOM
              64 CB ILE 208
                               38.421 19.627 56.174 1.00 44.50
             65 CG2 ILE 208
                                38.226 18.801 57.445 1.00 49.37
     ATOM
              66 CG1 ILE 208
                                37.766 20.993 56.385 1.00 42.73
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     ATOM
                                36.266 20.941 56.567 1.00 44.13
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             67 CD1 ILE 208
              68 C ILE 208
                              40.614 18.477 55.643 1.00 47.80
     ATOM
                               40.735 17.666 56.562 1.00 49.81
     ATOM
              69 O ILE 208
                                41.059 18.238 54.412 1.00 51.31
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              70 N GLY 209
                                41.728 16.983 54.107 1.00 46.85
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     ATOM
              71 CA GLY 209
             72 C GLY 209
73 O GLY 209
                                40.813 15.896 53.573 1.00 48.31
     ATOM
                                41.203 14.730 53.485 1.00 47.75
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              74 N HIS 210
                               39.582 16.274 53.237 1.00 46.79
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             75 CA HIS 210
                               38.622 15.326 52.686 1.00 47.34
     ATOM
                               37.200 15.739 53.068 1.00 49.39
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             76 CB HIS 210
     ATOM
     ATOM
              77 C HIS 210
                               38.796 15.350 51.162 1.00 45.47
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              78 O HIS 210
                               38.924 16.420 50.566 1.00 41.32
              79 N LYS 211
                               38.829 14.176 50.545 1.00 45.76
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             80 CA LYS 211
                                38.991 14.095 49.090 1.00 43.42
     ATOM
             81 CB LYS 211
                                39.892 12.910 48.715 1.00 46.72
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     ATOM
             82 CG LYS 211
                                41.210 12.815 49.497 1.00 56.48
     ATOM
                                42.068 14.089 49.486 1.00 60.93
     ATOM
              83 CD LYS 211
     ATOM
              84 CE LYS 211
                                42.562 14.496 48.103 1.00 61.95
     ATOM
              85 NZ LYS 211
                                41.485 15.024 47.218 1.00 69.93
             86 C LYS 211
                               37.609 13.917 48.473 1.00 35.68
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     ATOM
             87 O LYS 211
     ATOM
                               37.019 12.847 48.557 1.00 33.58
             88 N PRO 212
     ATOM
                               37.077 14.972 47.828 1.00 35.64
     ATOM
             89 CD PRO 212
                                37.654 16.304 47.584 1.00 38.60
     ATOM
             90 CA PRO 212
                                35.748 14.896 47.211 1.00 38.35
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     ATOM
             91 CB PRO 212
                                35.537 16.318 46.682 1.00 38.95
     ATOM
             92 CG PRO 212
                                36.409 17.156 47.604 1.00 42.00
     ATOM
             93 C PRO 212
                               35.635 13.865 46.096 1.00 38.78
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             94 O PRO 212
                               36.546 13.714 45.280 1.00 34.64
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             95 N GLU 213
                                34.517 13.153 46.077 1.00 40.31
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             96 CA GLU 213
                                34.256 12.160 45.049 1.00 43.87
     ATOM
     ATOM
             97 CB GLU 213
                                33.722 10.873 45.684 1.00 45.16
                                34.616 10.344 46.800 1.00 47.60
     ATOM
             98 CG GLU 213
             99 CD GLU 213
                                34,404 8.870 47.088 1.00 50.68
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             100 OE1 GLU 213
                                 33.240 8.416 47.072 1.00 59.18
     ATOM
                                 35.402 8.167 47.353 1.00 49.06
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     ATOM
             101 OE2 GLU 213
                                33.234 12.796 44.083 1.00 45.96
     ATOM
             102 C GLU 213
                                32.703 13.876 44.368 1.00 43.13
     ATOM
             103 O GLU 213
                                32,953 12.154 42.933 1.00 46.52
     ATOM
             104 N PRO 214
             105 CD PRO 214
                                 33.459 10.884 42.391 1.00 46.44
     ATOM
             106 CA PRO 214
                                 31.995 12.737 41.982 1.00 47.52
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	ATOM	107 CB PRO 214	32.040 11.750 40.813 1.00 45.40
	ATOM	108 CG PRO 214	33.445 11.181 40.913 1.00 49.89
	ATOM	109 C PRO 214	30.564 12.969 42.465 1.00 45.70
	ATOM	110 O PRO 214	29.972 12.112 43.121 1.00 44.49
5	ATOM	111 N THR 215	30.013 14.136 42.129 1.00 45.24
	ATOM	112 CA THR 215	28.629 14.447 42.483 1.00 49.36
	ATOM	113 CB THR 215	28.312 15.949 42.330 1.00 44.86
	ATOM	114 OG1 THR 215	28.253 16.285 40.942 1.00 52.26
	ATOM	115 CG2 THR 215	29.387 16.793 42.992 1.00 39.43
10	ATOM	116 C THR 215	27.791 13.673 41.464 1.00 52.51
	ATOM	117 O THR 215	28.326 13.192 40.465 1.00 53.48
	ATOM	118 N ASP 216	26.491 13.543 41.712 1.00 58.81
	ATOM	119 CA ASP 216	25.603 12.810 40.805 1.00 61.51
	ATOM	120 CB ASP 216	24.150 12.941 41.270 1.00 70.57
15	ATOM	121 CG ASP 216	23.902 12.257 42.595 1.00 78.07
	ATOM	122 OD1 ASP 216	24.042 11.018 42.660 1.00 82.31
	ATOM	123 OD2 ASP 216	23.572 12.962 43.571 1.00 86.55
	ATOM	124 C ASP 216	25.706 13.277 39.356 1.00 58.42
	ATOM	125 O ASP 216	25.695 12.464 38.429 1.00 56.85
20	ATOM	126 N GLU 217	25.798 14.587 39.167 1.00 54.92
	ATOM	127 CA GLU 217	25.905 15.156 37.833 1.00 53.37
	ATOM	128 CB GLU 217	25.861 16.682 37.906 1.00 51.02
	ATOM	129 C GLU 217	27.211 14.692 37.195 1.00 53.55
	ATOM	130 O GLU 217	27.239 14.301 36.027 1.00 54.33
25	ATOM	131 N GLU 218	28.290 14.726 37.975 1.00 49.20
	ATOM	132 CA GLU 218	29.593 14.310 37.486 1.00 45.94
	ATOM	133 CB GLU 218	30.674 14.601 38.530 1.00 43.43
	ATOM	134 CG GLU 218	30.787 16.069 38.878 1.00 40.86
	ATOM	135 CD GLU 218	31.930 16.347 39.826 1.00 39.88
30	ATOM	136 OE1 GLU 218	32.000 15.667 40.875 1.00 37.61
	ATOM	137 OE2 GLU 218	32.748 17.250 39.529 1.00 34.01
	ATOM	138 C GLU 218	29.624 12.838 37.101 1.00 44.71
	ATOM	139 O GLU 218	30.275 12.471 36.130 1.00 45.31
	ATOM	140 N TRP 219	28.935 11.991 37.863 1.00 44.02
35	ATOM	141 CA TRP 219	28.892 10.572 37.539 1.00 46.97
	ATOM	142 CB TRP 219	28.183 9.762 38.630 1.00 48.42
	ATOM	143 CG TRP 219	29.034 9.473 39.823 1.00 54.61
	ATOM	144 CD2 TRP 219	30.167 8.572 39.879 1.00 55.24
	ATOM	145 CE2 TRP 219	30.659 8.610 41.201 1.00 53.67
40	ATOM	146 CE3 TRP 219	30.795 7.745 38.938 1.00 54.55
	ATOM	147 CD1 TRP 219	28.902 10.000 41.074 1.00 55.75
	ATOM	148 NE1 TRP 219	29.868 9.491 41.912 1.00 54.43
	ATOM	149 CZ2 TRP 219	31.771 7.846 41.622 1.00 52.54
	ATOM	150 CZ3 TRP 219	31.912 6.975 39.353 1.00 55.17
45	ATOM	151 CH2 TRP 219	32.380 7.038 40.690 1.00 55.59
	ATOM	152 C TRP 219	28.167 10.356 36.216 1.00 47.32
	ATOM	153 O TRP 219	28.433 9.384 35.503 1.00 43.56
	ATOM	154 N GLU 220	27.247 11.259 35.898 1.00 49.91
	ATOM		26.497 11.155 34.655 1.00 53.57
50	ATOM	156 CB GLU 220	25.274 12.075 34.694 1.00 58.18

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            157 CG GLU 220
                                24.323 11.876 33.526 1.00 73.13
            158 CD GLU 220
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            159 OE1 GLU 220
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            160 OE2 GLU 220
                                22.839 13.545 32.701 1.00 82.78
     ATOM
            161 C GLU 220
                               27.419 11.534 33.497 1.00 50.51
     ATOM
            162 O GLU 220
                               27.399 10.899 32.443 1.00 49.94
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            163 N LEU 221
                               28.232 12.567 33.711 1.00 43.71
     ATOM
                                29.187 13.019 32.702 1.00 42.81
            164 CA LEU 221
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                               29.868 14.317 33.155 1.00 39.21
            165 CB LEU 221
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                                30.945 14.949 32.261 1.00 36.34
            166 CG LEU 221
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                                30.339 15.351 30.922 1.00 36.93
            167 CD1 LEU 221
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                                31.535 16.164 32.949 1.00 24.18
            168 CD2 LEU 221
     ATOM
                               30.234 11.928 32.505 1.00 43.46
            169 C LEU 221
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            170 O LEU 221
            171 N ILE 222
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15
            172 CA ILE 222
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     ATOM
            173 CB ILE 222
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            174 CG2 ILE 222
                               32.822 8.505 35.018 1.00 28.86
     ATOM
            175 CG1 ILE 222
                               32.813 10.918 35.745 1.00 33.33
     ATOM
                               33.111 10.646 37.199 1.00 34.85
            176 CD1 ILE 222
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     ATOM
            177 C ILE 222
                              31.139 9.098 32.781 1.00 34.26
     ATOM
                              31.877 8.427 32.070 1.00 31.90
            178 O ILE 222
     ATOM
            179 N LYS 223
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                                29.168 7.775 32.210 1.00 44.43
            180 CA LYS 223
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            181 CB LYS 223
                               27.696 7.733 32.635 1.00 50.81
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     ATOM
            182 CG LYS 223
                                26.845 6.693 31.929 1.00 62.51
     ATOM
                                25.379 6.856 32.313 1.00 72.22
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            183 CD LYS 223
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            184 CE LYS 223
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            186 C LYS 223
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            187 O LYS 223
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     ATOM
            188 N THR 224
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            189 CA THR 224
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            190 CB THR 224
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     ATOM
            191 OG1 THR 224
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            192 CG2 THR 224
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            193 C THR 224
                               30.333 9.433 28.234 1.00 39.96
     ATOM
     ATOM
            194 O THR 224
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            195 N VAL 225
                               31.303 10.123 28.833 1.00 38.02
            196 CA VAL 225
                                32.680 10.117 28.355 1.00 38.12
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     ATOM
            197 CB VAL 225
                                33.565 11.014 29.243 1.00 38.19
     ATOM
                                34.960 11.162 28.632 1.00 36.77
     ATOM
            198 CG1 VAL 225
            199 CG2 VAL 225
                                32.910 12.361 29.406 1.00 41.76
     ATOM
            200 C VAL 225
                               33.291 8.724 28.302 1.00 37.52
     ATOM
            201 O VAL 225
                               34.022 8.395 27.364 1.00 36.77
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     ATOM
            202 N THR 226
                               33.002 7.904 29.310 1.00 34.02
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     ATOM
            203 CA THR 226
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                                33.237 5.857 30.707 1.00 30.56
     ATOM
            204 CB THR 226
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            205 OG1 THR 226
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            206 CG2 THR 226
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            208 O THR 226
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           213 O GLU 227
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    ATOM 215 CA ALA 228
           216 CB ALA 228
                               32.285 8.746 24.256 1.00 28.25
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    ATOM 217 C ALA 228
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    ATOM 218 O ALA 228
           219 N HIS 229
                              34.404 6.611 24.843 1.00 33.58
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                              35.724 6.029 24.669 1.00 32.97
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            220 CA HIS 229
            221 CB HIS 229
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            222 CG HIS 229
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            223 CD2 HIS 229
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            224 ND1 HIS 229
    ATOM
           225 CE1 HIS 229
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                               39.556 4.147 26.332 1.00 31.27
           226 NE2 HIS 229
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    ATOM
           227 C HIS 229
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           228 O HIS 229
                              36.227 4.071 23.383 1.00 41.49
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                               33.964 1.726 26.196 1.00 44.68
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           232 CG1 VAL 230
                                33.865 0.208 26.041 1.00 39.39
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           233 CG2 VAL 230
                                34.576 2.075 27.540 1.00 42.18
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                              34.219 1.934 23.700 1.00 44.28
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            234 C VAL 230
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            235 O VAL 230
            236 N ALA 231
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                               32.580 2.403 21.961 1.00 47.84
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           238 CB ALA 231
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           240 O ALA 231
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    ATOM 243 CB THR 232
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    ATOM 245 CG2 THR 232
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    ATOM
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            252 OD1 ASN 233
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            253 ND2 ASN 233
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             273 O GLY 236
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            276 CB SER 237
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            277 C SER 237
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            278 O SER 237
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     ATOM 282 C HIS 238
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             286 CB TRP 239
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             288 CD2 TRP 239
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             289 CE2 TRP 239
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            291 CD1 TRP 239
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            292 NE1 TRP 239
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            293 CZ2 TRP 239
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     ATOM 294 CZ3 TRP 239
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     ATOM
            295 CH2 TRP 239
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            296 C TRP 239
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            297 O TRP 239
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             299 CA LYS 240
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     ATOM
             300 CB LYS 240
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             301 CG LYS 240
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     ATOM
             302 CD LYS 240
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     ATOM
             303 CE LYS 240
                                48.839 -8.515 26.573 1.00 71.31
     ATOM
             304 NZ LYS 240
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     ATOM
             305 C LYS 240
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            306 O LYS 240
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	ATOM	308 CA ASN 241	44.773 -12.089 21.750 1.00 67.53
	ATOM	309 CB ASN 241	43.503 -12.813 22.213 1.00 67.98
	ATOM	310 CG ASN 241	43.504 -13.096 23.704 1.00 70.19
5	ATOM	311 OD1 ASN 241	44.410 -13.744 24.227 1.00 71.37
	ATOM	312 ND2 ASN 241	42.483 -12.605 24.400 1.00 71.48
	ATOM	313 C ASN 241	44.621 -11.681 20.286 1.00 66.62
	ATOM	314 O ASN 241	44.882 -12.475 19.382 1.00 64.76
	ATOM	315 N LYS 242	44.196 -10.436 20.070 1.00 66.86
10	ATOM	316 CA LYS 242	43.989 -9.882 18.732 1.00 67.46
	ATOM	317 CB LYS 242	42.982 -8.731 18.799 1.00 67.93
	ATOM	318 CG LYS 242	41.601 -9.138 19.279 1.00 71.52
	ATOM	319 CD LYS 242	40.876 -9.986 18.246 1.00 74.32
	ATOM	320 CE LYS 242	40.449 -9.160 17.043 1.00 74.41
15	ATOM	321 NZ LYS 242	39.455 -8.120 17.436 1.00 74.44
	ATOM	322 C LYS 242	45.281 -9.367 18.097 1.00 66.28
	ATOM	323 O LYS 242	45.414 -9.334 16.874 1.00 67.61
	ATOM	324 N ARG 243	46.225 -8.961 18.938 1.00 64.19
	ATOM	325 CA ARG 243	47.497 -8.422 18.478 1.00 62.43
20	ATOM	326 CB ARG 243	48.376 -8.070 19.685 1.00 60.12
	ATOM	327 C ARG 243	48.261 -9.348 17.538 1.00 62.97
	ATOM	328 O ARG 243	48.585 -10.484 17.891 1.00 63.96
	ATOM	329 N LYS 244	48.531 -8.853 16.334 1.00 62.41
	ATOM	330 CA LYS 244	49.303 -9.593 15.339 1.00 61.57
25	ATOM	331 CB LYS 244	48.601 -9.607 13.972 1.00 63.68
25	ATOM	332 CG LYS 244	47.210 -10.231 13.970 1.00 71.29
	ATOM	333 CD LYS 244	46.666 -10.441 12.549 1.00 73.83
	ATOM	334 CE LYS 244	46.505 -9.139 11.767 1.00 74.71
	ATOM	335 NZ LYS 244	45.542 -8.199 12.407 1.00 73.32
30	ATOM	336 C LYS 244	50.613 -8.824 15.223 1.00 59.30
50	ATOM	337 O LYS 244	50.637 -7.716 14.686 1.00 56.34
	ATOM	338 N PHE 245	51.690 -9.405 15.744 1.00 57.06
	ATOM	339 CA PHE 245	52.996 -8.757 15.704 1.00 59.01
	ATOM	340 CB PHE 245	54.034 -9.588 16.467 1.00 59.62
35	ATOM	341 CG PHE 245	53.704 -9.783 17.934 1.00 66.60
J J	ATOM	342 CD1 PHE 245	52.656 -10.626 18.329 1.00 67.17
	ATOM	343 CD2 PHE 245	54.427 -9.096 18.918 1.00 69.25
	ATOM	344 CE1 PHE 245	52.320 -10.789 19.699 1.00 69.92
	ATOM	345 CE2 PHE 245	54.111 -9.240 20.294 1.00 70.50
40	ATOM	346 CZ PHE 245	53.051 -10.091 20.686 1.00 70.89
40	ATOM	347 C PHE 245	53.463 -8.537 14.272 1.00 60.68
	ATOM	348 O PHE 245	53.433 -9.455 13.447 1.00 62.37
			53.880 -7.311 13.976 1.00 60.10
	ATOM		54.359 -6.968 12.642 1.00 59.44
4.5	ATOM	350 CA LEU 246	
45	ATOM	351 CB LEU 246	54.654 -5.464 12.560 1.00 57.43
	ATOM	352 CG LEU 246	54.937 -4.851 11.183 1.00 54.41 53.681 -4.931 10.320 1.00 52.43
	ATOM	353 CD1 LEU 246	
	ATOM	354 CD2 LEU 246	55.358 -3.398 11.343 1.00 51.69 55.638 -7.772 12.425 1.00 62.05
50	ATOM	355 C LEU 246	
50	ATOM	356 O LEU 246	56.447 -7.923 13.346 1.00 59.85

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             358 CD PRO 247
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             359 CA PRO 247
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            377 OD2 ASP 249
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            382 CB ILE 250
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            383 CG2 ILE 250
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            385 CD1 ILE 250
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            387 O ILE 250
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            404 C ALA 253
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            431 O LYS 263
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            438 CG2 VAL 264
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            444 CG ASP 265
            445 OD1 ASP 265
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            446 OD2 ASP 265
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            453 CD1 LEU 266
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            454 CD2 LEU 266
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            459 CB GLU 267
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            460 CG GLU 267
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            473 CB PHE 269
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            475 CD1 PHE 269
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            477 CE1 PHE 269
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            478 CE2 PHE 269
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                              52.903 3.622 6.443 1.00 52.15
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            481 O PHE 269
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            495 NE2 HIS 271
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                               51.472 1.321 8.537 1.00 41.34
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                               50.946 2.316 9.462 1.00 39.44
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                                52.076 3.215 9.976 1.00 36.67
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                                53.167 2.475 10.749 1.00 33.39
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            502 CD1 PHE 272
            503 CD2 PHE 272
                                52.934 1.216 11.311 1.00 38.28
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                                55.454 2.418 11.633 1.00 38.26
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     ATOM
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            505 CE2 PHE 272
                                53,961 0.538 12.047 1.00 43.28
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                               55.225 1.146 12.207 1.00 39.74
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                               49.857 3.183 8.822 1.00 40.75
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                               48.784 3.361 9.394 1.00 35.51
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                               50.136 3.714 7.635 1.00 41.64
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            510 CA THR 273
                                49.170 4.561 6.938 1.00 45.97
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            511 CB THR 273
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            512 OG1 THR 273
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            514 C THR 273
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            515 O THR 273
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            519 C LYS 274
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            520 O LYS 274
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            523 CB ILE 275
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            529 N ILE 276
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            535 C ILE 276
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            536 O ILE 276
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            540 OG1 THR 277
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            546 CA PRO 278
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            550 O PRO 278
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            551 N ALA 279
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            552 CA ALA 279
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            553 CB ALA 279
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                                43.836 5.135 13.949 1.00 30.56
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            555 O ALA 279
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            560 CG1 ILE 280
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            563 O ILE 280
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            569 C THR 281
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            570 O THR 281
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            571 N ARG 282
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            573 CB ARG 282
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            574 CG ARG 282
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            575 CD ARG 282
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            576 NE ARG 282
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            577 CZ ARG 282
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            578 NH1 ARG 282
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            579 NH2 ARG 282
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                               37.006 7.886 17.884 1.00 36.03
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            581 O ARG 282
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	ATOM	583 CA VAL 283	38.952 9.815 17.532 1.00 30.16
	ATOM	584 CB VAL 283	40.298 10.524 17.224 1.00 29.00
	ATOM	585 CG1 VAL 283	40.448 11.777 18.076 1.00 28.64
5	ATOM	586 CG2 VAL 283	41.448 9.577 17.487 1.00 28.28
	ATOM	587 C VAL 283	37.801 10.787 17.292 1.00 32.50
	ATOM	588 O VAL 283	37.284 11.388 18.236 1.00 33.48
	ATOM	589 N VAL 284	37.403 10.945 16.028 1.00 30.96
	ATOM	590 CA VAL 284	36.293 11.838 15.694 1.00 29.14
10	ATOM	591 CB VAL 284	36.138 12.023 14.158 1.00 31.27
	ATOM	592 CG1 VAL 284	34.990 12.985 13.868 1.00 24.21
	ATOM	593 CG2 VAL 284	37.450 12.565 13.554 1.00 30.51
	ATOM	594 C VAL 284	34.995 11.260 16.258 1.00 28.89
	ATOM	595 O VAL 284	34.146 12.005 16.743 1.00 27.29
15	ATOM	596 N ASP 285	34.845 9.937 16.208 1.00 28.76
	ATOM	597 CA ASP 285	33.639 9.307 16.738 1.00 35.32
	ATOM	598 CB ASP 285	33.627 7.792 16.459 1.00 33.29
	ATOM	599 CG ASP 285	33.523 7.471 14.971 1.00 38.15
	ATOM	600 OD1 ASP 285	32.729 8.139 14.276 1.00 34.70
20	ATOM	601 OD2 ASP 285	34.209 6.532 14.504 1.00 34.43
	ATOM	602 C ASP 285	33.531 9.553 18.248 1.00 36.70
	ATOM	603 O ASP 285	32.431 9.685 18.786 1.00 37.96
	ATOM	604 N PHE 286	34.679 9.624 18.916 1.00 35.96
	ATOM	605 CA PHE 286	34.736 9.869 20.349 1.00 37.10
25	ATOM	606 CB PHE 286	36.187 9.777 20.845 1.00 37.97
	ATOM	607 CG PHE 286	36.377 10.219 22.283 1.00 36.50
	ATOM	608 CD1 PHE 286	35.815 9.490 23.340 1.00 36.75
	ATOM	609 CD2 PHE 286	37.100 11.381 22.575 1.00 33.83
	ATOM	610 CE1 PHE 286	35.966 9.917 24.685 1.00 39.55
30	ATOM	611 CE2 PHE 286	37.265 11.831 23.911 1.00 38.08
	ATOM	612 CZ PHE 286	36.696 11.092 24.972 1.00 34.44
	ATOM	613 C PHE 286	34.179 11.249 20.665 1.00 36.83
	ATOM	614 O PHE 286	33.292 11.401 21.518 1.00 35.61
	ATOM	615 N ALA 287	34.696 12.255 19.968 1.00 37.33
35	ATOM	616 CA ALA 287	34.266 13.631 20.171 1.00 36.34
	ATOM	617 CB ALA 287	35.118 14.565 19.325 1.00 36.40
	ATOM	618 C ALA 287	32.785 13.840 19.861 1.00 38.76
	ATOM	619 O ALA 287	32.121 14.641 20.525 1.00 41.98
	ATOM	620 N LYS 288	32.267 13.130 18.862 1.00 38.28
40	ATOM	621 CA LYS 288	30.856 13.268 18.499 1.00 45.26
	ATOM	622 CB LYS 288	30.541 12.534 17.188 1.00 48.35
	ATOM	623 CG LYS 288	31.159 13.158 15.951 1.00 51.43
	ATOM	624 CD LYS 288	30.556 12.589 14.665 1.00 60.23
	ATOM	625 CE LYS 288	30.848 11.107 14.479 1.00 62.81
45	ATOM	626 NZ LYS 288	32.312 10.852 14.392 1.00 64.69
	ATOM	627 C LYS 288	29.913 12.763 19.586 1.00 43.31
	ATOM	628 O LYS 288	28.791 13.253 19.707 1.00 45.66
	ATOM	629 N LYS 289	30.367 11.789 20.371 1.00 41.70
	ATOM	630 CA LYS 289	29.548 11.235 21.443 1.00 40.67
50	ATOM	631 CB LYS 289	29.984 9.806 21.767 1.00 42.25

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             634 CE LYS 289
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            635 NZ LYS 289
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            636 C LYS 289
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            637 O LYS 289
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            641 CG LEU 290
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            643 CD2 LEU 290
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            644 C LEU 290
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                               28.279 15.500 24.137 1.00 40.27
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            647 CD PRO 291
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            649 CB PRO 291
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            657 SD MET 292
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            658 CE MET 292
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                                33.117 17.902 20.070 1.00 42.78
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            667 CE1 PHE 293
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            671 O PHE 293
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            673 CA CYS 294
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            679 CA GLU 295
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            681 CG GLU 295
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            685 C GLU 295
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            704 CB CYS 298
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            724 O ASP 300
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            726 CA GLN 301
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            727 CB GLN 301
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            728 CG GLN 301
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            729 CD GLN 301
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                                31.074 20.527 14.673 1.00 45.73
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                                30.450 20.363 16.824 1.00 46.13
            731 NE2 GLN 301
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	ATOM	733 O GLN 301	36.975 19.850 15.601 1.00 45.02
	ATOM	734 N ILE 302	36.523 21.441 14.077 1.00 41.01
	ATOM	735 CA ILE 302	37.607 21.029 13.189 1.00 40.23
5	ATOM	736 CB ILE 302	37.580 21.798 11.825 1.00 39.52
	ATOM	737 CG2 ILE 302	38.724 21.308 10.931 1.00 31.98
	ATOM	738 CG1 ILE 302	36.230 21.607 11.119 1.00 40.77
	ATOM	739 CD1 ILE 302	35.895 20.166 10.733 1.00 45.43
	ATOM	740 C ILE 302	38.948 21.322 13.869 1.00 38.58
10	ATOM	741 O ILE 302	39.811 20.452 13.938 1.00 40.81
	ATOM	742 N ILE 303	39.110 22.547 14.364 1.00 37.50
	ATOM	743 CA ILE 303	40.343 22.958 15.030 1.00 39.33
	ATOM	744 CB ILE 303	40.263 24.442 15.501 1.00 39.06
	ATOM	745 CG2 ILE 303	41.525 24.822 16.279 1.00 36.19
15	ATOM	746 CG1 ILE 303	40.103 25.358 14.280 1.00 40.15
	ATOM	747 CD1 ILE 303	39.972 26.846 14.602 1.00 36.93
	ATOM	748 C ILE 303	40.676 22.061 16.222 1.00 36.49
	ATOM	749 O ILE 303	41.818 21.623 16.378 1.00 36.58
	ATOM	750 N LEU 304	39.674 21.788 17.057 1.00 32.91
20	ATOM	751 CA LEU 304	39.851 20.940 18.234 1.00 27.55
	ATOM	752 CB LEU 304	38.546 20.875 19.026 1.00 22.35
	ATOM	753 CG LEU 304	38.472 21.629 20.361 1.00 26.88
	ATOM	754 CD1 LEU 304	39.096 22.998 20.275 1.00 24.82
	ATOM	755 CD2 LEU 304	37.024 21.728 20.787 1.00 23.69
25	ATOM	756 C LEU 304	40.313 19.534 17.855 1.00 28.05
	ATOM	757 O LEU 304	41.277 19.013 18.429 1.00 24.68
	ATOM	758 N LEU 305	39.637 18.929 16.882 1.00 26.34
	ATOM	759 CA LEU 305	39.997 17.588 16.436 1.00 30.91
	ATOM	760 CB LEU 305	38.937 17.055 15.466 1.00 32.50
30	ATOM	761 CG LEU 305	37.585 16.757 16.132 1.00 33.36
	ATOM	762 CD1 LEU 305	36.557 16.439 15.079 1.00 33.87
	ATOM	763 CD2 LEU 305	37.733 15.581 17.101 1.00 31.72
	ATOM	764 C LEU 305	41.381 17.523 15.796 1.00 29.76
	ATOM	765 O LEU 305	42.109 16.553 15.990 1.00 29.33
35	ATOM	766 N LYS 306	41.754 18.554 15.048 1.00 29.72
	ATOM	767 CA LYS 306	43.065 18.569 14.409 1.00 34.28
	ATOM	768 CB LYS 306	43.122 19.673 13.345 1.00 35.98
	ATOM	769 CG LYS 306	42.140 19.465 12.206 1.00 43.35
	ATOM	770 CD LYS 306	42.195 20.583 11.170 1.00 51.50
40	ATOM	771 CE LYS 306	43.532 20.639 10.446 1.00 53.26
	ATOM	772 NZ LYS 306	43.522 21.702 9.409 1.00 59.61
	ATOM	773 C LYS 306	44.183 18.777 15.434 1.00 35.25
	ATOM	774 O LYS 306	45.312 18.332 15.231 1.00 33.95
	ATOM	775 N GLY 307	43.853 19.446 16.536 1.00 35.79
45	ATOM	776 CA GLY 307	44.836 19.700 17.576 1.00 34.59
	ATOM	777 C GLY 307	45.075 18.562 18.559 1.00 33.80
	ATOM	778 O GLY 307	46.200 18.360 19.008 1.00 31.59
	ATOM	779 N CYS 308	44.030 17.806 18.880 1.00 31.15
	ATOM	780 CA CYS 308	44.153 16.712 19.839 1.00 29.04
50	ATOM	781 CB CYS 308	42.929 16.667 20.750 1.00 27.59

	ATOM	782 SG CYS 308	41,452 15.974 19.941 1.00 30.50
	ATOM	783 C CYS 308	44.289 15.339 19.208 1.00 30.59
	ATOM	784 O CYS 308	44.609 14.374 19.899 1.00 33.77
	ATOM	785 N CYS 309	44.053 15.247 17.907 1.00 28.46
5	ATOM	786 CA CYS 309	44.099 13.961 17.219 1.00 30.10
	ATOM	787 CB CYS 309	43.983 14.161 15.706 1.00 33.43
	ATOM	788 SG CYS 309	43.761 12.613 14.819 1.00 35.20
	ATOM	789 C CYS 309	45.301 13.071 17.524 1.00 27.72
	ATOM	790 O CYS 309	45.135 11.907 17.913 1.00 27.69
10	ATOM	791 N MET 310	46.508 13.594 17.339 1.00 26.15
	ATOM	792 CA MET 310	47.700 12.798 17.605 1.00 26.06
	ATOM	793 CB MET 310	48.928 13.439 16.951 1.00 25.32
	ATOM	794 CG MET 310	50.207 12.648 17.132 1.00 24.08
	ATOM	795 SD MET 310	50.101 10.991 16.423 1.00 27.71
15	ATOM	796 CE MET 310	51.674 10.307 16.934 1.00 28.50
	ATOM	797 C MET 310	47.941 12.612 19.113 1.00 25.94
	ATOM	798 O MET 310	48.592 11.653 19.526 1.00 28.09
	ATOM	799 N GLU 311	47.405 13.522 19.923 1.00 25.39
	ATOM	800 CA GLU 311	47.560 13.445 21.370 1.00 27.03
20	ATOM	801 CB GLU 311	47.099 14.748 22.030 1.00 24.39
	ATOM	802 CG GLU 311	47.610 15.999 21.331 1.00 26.00
	ATOM	803 CD GLU 311	47.292 17.271 22.084 1.00 23.95
	ATOM	804 OE1 GLU 311	46.182 17.379 22.640 1.00 19.72
	ATOM	805 OE2 GLU 311	48.150 18.181 22.088 1.00 26.51
25	ATOM	806 C GLU 311	46.727 12.272 21.902 1.00 27.51
	ATOM	807 O GLU 311	47.152 11.552 22.807 1.00 29.67
	ATOM	808 N ILE 312	45.547 12.086 21.326 1.00 26.82
	ATOM	809 CA ILE 312	44.661 11.001 21.724 1.00 25.71
	ATOM	810 CB ILE 312	43.194 11.296 21.304 1.00 23.35
30	ATOM	811 CG2 ILE 312	42.301 10.068 21.583 1.00 20.27
	ATOM	812 CG1 ILE 312	42.690 12.534 22.062 1.00 20.88
	ATOM	813 CD1 ILE 312	41.244 12.961 21.755 1.00 18.15
	ATOM	814 C ILE 312	45.116 9.665 21.132 1.00 27.91
	ATOM	815 O ILE 312	45.064 8.628 21.804 1.00 28.96
35	ATOM	816 N MET 313	45.582 9.683 19.886 1.00 27.66
	ATOM	817 CA MET 313	46.045 8.447 19.257 1.00 30.18
	ATOM	818 CB MET 313	46.386 8.662 17.771 1.00 36.89
	ATOM	819 CG MET 313	45.186 8.938 16.861 1.00 37.95
	ATOM	820 SD MET 313	45.624 8.943 15.096 1.00 42.38
40	ATOM	821 CE MET 313	46.724 10.319 14.999 1.00 40.68
	ATOM	822 C MET 313	47.264 7.897 19.975 1.00 27.43
	ATOM	823 O MET 313	47.351 6.690 20.219 1.00 28.61
	ATOM	824 N SER 314	48.202 8.776 20.318 1.00 24.88
	ATOM	825 CA SER 314	49.416 8.352 21.011 1.00 27.98
45	ATOM	826 CB SER 314	50.420 9.511 21.118 1.00 29.64
	ATOM	827 OG SER 314	49.912 10.560 21.911 1.00 43.44
	ATOM	828 C SER 314	49.082 7.818 22.402 1.00 22.30
	ATOM	829 O SER 314	49.737 6.895 22.892 1.00 24.18
	ATOM	830 N LEU 315	48.070 8.395 23.039 1.00 23.99
50	ATOM	831 CA LEU 315	47.646 7.918 24.365 1.00 25.07

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46.580 8.842 24.965 1.00 19.11
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            833 CG LEU 315
    ATOM
                                46.872 8.076 27.362 1.00 18.92
            834 CD1 LEU 315
    ATOM
                                44.848 9.401 26.655 1.00 12.93
            835 CD2 LEU 315
    ATOM
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    ATOM
            836 C LEU 315
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    ATOM
            837 O LEU 315
            838 N ARG 316
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    ATOM
    ATOM
            840 CB ARG 316
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                               43,340 5.929 22.253 1.00 22.00
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            841 CG ARG 316
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    ATOM
            842 CD ARG 316
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    ATOM
            843 NE ARG 316
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            844 CZ ARG 316
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            845 NH1 ARG 316
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    ATOM
            846 NH2 ARG 316
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    ATOM
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            847 C ARG 316
                              46.612 3.949 22.682 1.00 28.09
    ATOM
                               46.399 2.790 23.027 1.00 32.41
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25
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    ATOM
            857 C ALA 318
            858 O ALA 318
859 N VAL 319
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     ATOM 860 CA VAL 319
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    ATOM 861 CB VAL 319
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                               46.759 4.324 28.136 1.00 29.96
            862 CG1 VAL 319
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                               45.773 2.936 26.322 1.00 31.70
    ATOM 863 CG2 VAL 319
                               47.970 0.955 26.764 1.00 40.01
    ATOM 864 C VAL 319
    ATOM 865 O VAL 319
ATOM 866 N ARG 320
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                               48.460 0.644 25.565 1.00 38.64
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    ATOM 867 CA ARG 320
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                               47.764 -0.751 23.674 1.00 37.26
    ATOM 868 CB ARG 320
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            869 CG ARG 320
     ATOM
            870 CD ARG 320
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    ATOM
            871 NE ARG 320
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    ATOM
            872 CZ ARG 320
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     ATOM
                                44.119 0.713 20.300 1.00 49.08
            873 NH1 ARG 320
     ATOM
           874 NH2 ARG 320
                                42.206 -0.058 21.326 1.00 59.59
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                               49.852 -1.247 24.930 1.00 42.14
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            875 C ARG 320
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     ATOM 876 O ARG 320
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                               50.712 -0.772 25.822 1.00 42.04
     ATOM 877 N TYR 321
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     ATOM 878 CA TYR 321
     ATOM 879 CB TYR 321
                               52.971 -0.133 26.529 1.00 38.01
    ATOM 880 CG TYR 321
                               54.416 -0.579 26.734 1.00 37.94
    ATOM 881 CD1 TYR 321
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	ATOM	882 CE1 TYR 321	56.581 -1.297 25.813 1.00 34.49
	ATOM	883 CD2 TYR 321	54.892 -0.894 28.016 1.00 28.03
•	ATOM	884 CE2 TYR 321	56.194 -1.411 28.207 1.00 32.69
	ATOM	885 CZ TYR 321	57.026 -1.614 27.103 1.00 35.18
5	ATOM	886 OH TYR 321	58.289 -2.158 27.288 1.00 39.48
	ATOM	887 C TYR 321	52.189 -2.515 26.629 1.00 45.51
	ATOM	888 O TYR 321	51.571 -2.662 27.687 1.00 48.02
	ATOM	889 N ASP 322	52.945 -3.471 26.095 1.00 44.56
	ATOM	890 CA ASP 322	53.129 -4.764 26.753 1.00 45.86
10	ATOM	891 CB ASP 322	52,697 -5.899 25.816 1.00 46.64
	ATOM	892 C ASP 322	54.606 -4.910 27.098 1.00 45.82
	ATOM	893 O ASP 322	55.434 -5.109 26.214 1.00 45.38
	ATOM	894 N PRO 323	54.962 -4.803 28.393 1.00 46.53
	ATOM	895 CD PRO 323	54.123 -4.541 29.572 1.00 47.16
15	ATOM	896 CA PRO 323	56.366 -4.932 28.805 1.00 46.63
10	ATOM	897 CB PRO 323	56.293 -4.667 30.308 1.00 43.95
	ATOM	898 CG PRO 323	54.926 -5.223 30.655 1.00 43.93
	ATOM	899 C PRO 323	56.993 -6.285 28.478 1.00 48.34
	ATOM	900 O PRO 323	58.217 -6.407 28.379 1.00 50.84
20	ATOM	901 N GLU 324	56.149 -7.301 28.315 1.00 52.39
	ATOM	902 CA GLU 324	56.621 -8.646 28.005 1.00 55.85
	ATOM	903 CB GLU 324	55.453 -9.633 28.048 1.00 55.54
	ATOM	904 C GLU 324	57.283 -8.670 26.632 1.00 54.94
	ATOM	905 O GLU 324	58.460 -9.013 26.502 1.00 59.81
25	ATOM	906 N SER 325	56.522 -8.299 25.611 1.00 52.95
	ATOM	907 CA SER 325	57.021 -8.269 24.244 1.00 50.10
	ATOM	908 CB SER 325	55.889 -8.613 23.279 1.00 48.23
	ATOM	909 OG SER 325	54.788 -7.749 23.471 1.00 48.71
	ATOM	910 C SER 325	57.608 -6.908 23.879 1.00 50.61
30	ATOM	911 O SER 325	58.194 -6.743 22.808 1.00 52.19
	ATOM	912 N GLU 326	57.450 -5.939 24.786 1.00 45.64
	ATOM	913 CA GLU 326	57.938 -4.579 24.588 1.00 43.35
	ATOM	914 CB GLU 326	59.469 -4.562 24.587 1.00 42.74
	ATOM	915 CG GLU 326	60.053 -5.016 25.909 1.00 50.32
35	ATOM	916 CD GLU 326	61.565 -5.067 25.907 1.00 56.34
•	ATOM	917 OE1 GLU 326	62.139 -5.407 26.966 1.00 59.31
	ATOM	918 OE2 GLU 326	62.178 -4.774 24.856 1.00 55.74
	ATOM	919 C GLU 326	57.397 -3.993 23.291 1.00 40.23
	ATOM	920 O GLU 326	58.145 -3.474 22.465 1.00 40.44
40	ATOM	921 N THR 327	56.080 -4.079 23.127 1.00 35.90
	ATOM	922 CA THR 327	55.427 -3.573 21.936 1.00 37.29
	ATOM	923 CB THR 327	54.983 -4.717 21.008 1.00 37.63
	ATOM	924 OG1 THR 327	53.994 -5.503 21.674 1.00 38.12
	ATOM	925 CG2 THR 327	56,165 -5.609 20.635 1.00 39.90
45	ATOM	926 C THR 327	54.170 -2.780 22.282 1.00 39.49
	ATOM	927 O THR 327	53.603 -2.930 23.364 1.00 40.50
	ATOM	928 N LEU 328	53.758 -1.933 21.347 1.00 36.64
	ATOM	929 CA LEU 328	52.544 -1.136 21.480 1.00 37.73
	ATOM	930 CB LEU 328	52.791 0.340 21.127 1.00 37.78
50	ATOM	931 CG LEU 328	53.667 1.257 21.982 1.00 36.26

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             933 CD2 LEU 328
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            938 CB THR 329
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            940 CG2 THR 329
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             946 CG LEU 330
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            953 CB ASN 331
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            955 OD1 ASN 331
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            956 ND2 ASN 331
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            966 CG GLU 333
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            974 CB MET 334
     ATOM
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            975 CG MET 334
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     ATOM
            979 O MET 334
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     ATOM
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            981 CA ALA 335
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     ATOM
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     ATOM
            983 C ALA 335
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            984 O ALA 335
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            985 N VAL 336
                               55.016 -2.926 16.783 1.00 42.35
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            986 CA VAL 336
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     ATOM
            987 CB VAL 336
            988 CG1 VAL 336
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     ATOM 989 CG2 VAL 336
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            994 CB THR 337
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            995 OG1 THR 337
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     ATOM
            996 CG2 THR 337
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     ATOM 998 O THR 337
                               58.312 -0.218 17.473 1.00 34.06
     ATOM 999 N ARG 338
                               59.655 -0.489 19.268 1.00 37.61
     ATOM 1000 CA ARG 338
                                60.171 0.876 19.268 1.00 38.68
                                61.177 1.041 20.424 1.00 35.95
     ATOM 1001 CB ARG 338
20
     ATOM 1002 CG ARG 338
                                61.804 2.434 20.570 1.00 38.83
                                62.791 2.462 21.749 1.00 35.88
    ATOM 1003 CD ARG 338
                                62.114 2.277 23.035 1.00 37.42
     ATOM 1004 NE ARG 338
     ATOM 1005 CZ ARG 338
                                61.858 3.256 23.902 1.00 30.20
25
    ATOM 1006 NH1 ARG 338
                                62.224 4.501 23.636 1.00 27.98
                                 61.213 2.992 25.025 1.00 27.40
     ATOM 1007 NH2 ARG 338
     ATOM 1008 C ARG 338
                               60.843 1.158 17.925 1.00 38.09
     ATOM 1009 O ARG 338
                               60.529 2.142 17.251 1.00 34.12
    ATOM 1010 N GLY 339
                               61.755 0.267 17.535 1.00 41.25
    ATOM 1011 CA GLY 339
                                62.475 0.416 16.282 1.00 41.35
30
    ATOM 1012 C GLY 339
                               61.594 0.463 15.046 1.00 41.23
    ATOM 1013 O GLY 339
                               61.811 1.288 14.159 1.00 38.30
    ATOM 1014 N GLN 340
                               60.594 -0.414 14.982 1.00 38.58
                                59.704 -0.449 13.826 1.00 40.79
     ATOM 1015 CA GLN 340
    ATOM 1016 CB GLN 340
                                58.757 -1.651 13.911 1.00 40.82
35
    ATOM 1017 CG GLN 340
                                59.450 -2.995 13.944 1.00 41.10
    ATOM 1018 CD GLN 340
                                58.468 -4.144 13.890 1.00 48.84
    ATOM 1019 OE1 GLN 340
                                57.529 -4.208 14.679 1.00 50.53
    ATOM 1020 NE2 GLN 340
                                58.685 -5.068 12.959 1.00 54.25
40
    ATOM 1021 C GLN 340
                               58.884 0.822 13.679 1.00 41.50
    ATOM 1022 O GLN 340
                               58.725 1.342 12.576 1.00 42.72
    ATOM 1023 N LEU 341
                               58.360 1.324 14.795 1.00 42.00
                                57.546 2.532 14.775 1.00 38.10
    ATOM 1024 CA LEU 341
    ATOM 1025 CB LEU 341
                                56.868 2.740 16.133 1.00 36.66
45
    ATOM 1026 CG LEU 341
                                55.886 3.914 16.267 1.00 39.94
    ATOM 1027 CD1 LEU 341
                                54.711 3.741 15.311 1.00 34.98
    ATOM 1028 CD2 LEU 341
                                55.389 3.989 17.700 1.00 40.95
    ATOM 1029 C LEU 341
                               58.404 3.743 14.423 1.00 36.37
    ATOM 1030 O LEU 341
                               57.980 4.620 13.668 1.00 37.89
    ATOM 1031 N LYS 342
                               59.616 3.777 14.969 1.00 33.29
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ATOM 1032 CA LYS 342
                                60.542 4.872 14.723 1.00 35.17
                                61.801 4.687 15.582 1.00 34.97
     ATOM 1033 CB LYS 342
                                62.764 5.863 15.519 1.00 40.00
     ATOM 1034 CG LYS 342
     ATOM 1035 CD LYS 342
                                63.868 5.739 16.555 1.00 34.48
     ATOM 1036 CE LYS 342
                                64.709 7.001 16.596 1.00 37.54
     ATOM 1037 NZ LYS 342
                                65.716 6.972 17.689 1.00 42.32
     ATOM 1038 C LYS 342
                               60.928 4.970 13.235 1.00 38.29
     ATOM 1039 O LYS 342
                               60.621 5.963 12.569 1.00 36.23
     ATOM 1040 N ASN 343
                               61.585 3.932 12.721 1.00 39.25
     ATOM 1041 CA ASN 343
                                62.014 3.903 11.328 1.00 40.19
10
     ATOM 1042 CB ASN 343
                                62.808 2.627 11.050 1.00 37.96
     ATOM 1043 CG ASN 343
                                63.937 2.429 12.027 1.00 39.22
                                64.648 3.376 12.374 1.00 42.37
     ATOM 1044 OD1 ASN 343
     ATOM 1045 ND2 ASN 343
                                64.125 1.197 12.471 1.00 42.19
     ATOM 1046 C ASN 343
                               60.831 3.997 10.368 1.00 40.12
15
     ATOM 1047 O ASN 343
                               60.991 4.371 9.208 1.00 36.01
     ATOM 1048 N GLY 344
                               59.645 3.665 10.868 1.00 40.95
     ATOM 1049 CA GLY 344
                                58.439 3.721 10.057 1.00 39.25
     ATOM 1050 C GLY 344
                               57.947 5.131 9.772 1.00 38.26
20
     ATOM 1051 O GLY 344
                               56.971 5.308 9.044 1.00 35.69
     ATOM 1052 N GLY 345
                               58.604 6.135 10.359 1.00 35.89
     ATOM 1053 CA GLY 345
                                58.212 7.510 10.110 1.00 34.00
     ATOM 1054 C GLY 345
                               58.050 8.444 11.300 1.00 38.64
     ATOM 1055 O GLY 345
                               57.902 9.652 11.116 1.00 38.14
25
     ATOM 1056 N LEU 346
                               58.085 7.912 12.520 1.00 39.52
     ATOM 1057 CA LEU 346
                                57.904 8.761 13.692 1.00 36.05
     ATOM 1058 CB LEU 346
                                57.039 8.048 14.738 1.00 35.72
     ATOM 1059 CG LEU 346
                                55.561 7.864 14.371 1.00 34.89
     ATOM 1060 CD1 LEU 346
                                54.850 7.132 15.494 1.00 44.09
30
     ATOM 1061 CD2 LEU 346
                                54.903 9.213 14.146 1.00 34.84
     ATOM 1062 C LEU 346
                               59.189 9.264 14.339 1.00 33.52
     ATOM 1063 O LEU 346
                               59.171 10.257 15.066 1.00 35.58
     ATOM 1064 N GLY 347
                               60.299 8.595 14.067 1.00 30.47
     ATOM 1065 CA GLY 347
                                61.559 9.017 14.661 1.00 33.01
35
    ATOM 1066 C GLY 347
                               61.504 9.069 16.182 1.00 30.72
    ATOM 1067 O GLY 347
                               60.967 8.160 16.812 1.00 30.89
    ATOM 1068 N VAL 348
                               62.051 10.132 16.765 1.00 31.30
    ATOM 1069 CA VAL 348
                                62.084 10.291 18.221 1.00 31.27
    ATOM 1070 CB VAL 348
                                62.843 11.612 18.620 1.00 31.66
40
    ATOM 1071 CG1 VAL 348
                                62.071 12.841 18.146 1.00 20.19
    ATOM 1072 CG2 VAL 348
                                63.080 11.651 20.118 1.00 24.77
    ATOM 1073 C VAL 348
                               60.683 10.273 18.855 1.00 33.84
    ATOM 1074 O VAL 348
                               60.546 10.034 20.050 1.00 29.99
    ATOM 1075 N VAL 349
                               59.649 10.518 18.049 1.00 33.31
45
    ATOM 1076 CA VAL 349
                                58.270 10.495 18.538 1.00 32.23
    ATOM 1077 CB VAL 349
                                57.279 10.911 17.415 1.00 32.59
    ATOM 1078 CG1 VAL 349
                                55.837 10.678 17.838 1.00 33.68
    ATOM 1079 CG2 VAL 349
                                57.474 12.378 17.103 1.00 32.30
    ATOM 1080 C VAL 349
                               57.931 9.094 19.050 1.00 34.91
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    ATOM 1081 O VAL 349
                               57.133 8.932 19.980 1.00 33.73
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58.551 8.081 18.444 1.00 32.81
    ATOM 1082 N SER 350
                               58.335 6.704 18.853 1.00 30.10
    ATOM 1083 CA SER 350
                               59.041 5.746 17.904 1.00 24.95
    ATOM 1084 CB SER 350
                               58.943 4.417 18.387 1.00 23.16
    ATOM 1085 OG SER 350
                               58.863 6.486 20.266 1.00 31.59
    ATOM 1086 C SER 350
                               58.207 5.845 21.086 1.00 37.62
    ATOM 1087 O SER 350
                               60.055 7.007 20.546 1.00 28.60
    ATOM 1088 N ASP 351
    ATOM 1089 CA ASP 351
                               60.652 6.863 21.867 1.00 29.82
                               62.048 7.491 21.919 1.00 27.49
    ATOM 1090 CB ASP 351
    ATOM 1091 CG ASP 351
                               63.030 6.806 21.000 1.00 30.22
10
    ATOM 1092 OD1 ASP 351
                                63,411 7,412 19,974 1,00 32,61
    ATOM 1093 OD2 ASP 351
                                63.422 5.661 21.301 1.00 30.02
    ATOM 1094 C ASP 351
                               59.785 7.548 22.913 1.00 30.63
                               59.632 7.055 24.027 1.00 29.54
    ATOM 1095 O ASP 351
                               59.222 8.692 22.537 1.00 25.33
    ATOM 1096 N ALA 352
15
    ATOM 1097 CA ALA 352
                                58.390 9.464 23.432 1.00 28.59
                                58.011 10.798 22.788 1.00 20.95
    ATOM 1098 CB ALA 352
                               57.136 8.695 23.831 1.00 29.69
    ATOM 1099 C ALA 352
                               56.711 8.753 24.982 1.00 30.36
    ATOM 1100 O ALA 352
    ATOM 1101 N ILE 353
                              56.557 7.979 22.876 1.00 27.63
20
    ATOM 1102 CA ILE 353
                               55.345 7.227 23.129 1.00 27.55
    ATOM 1103 CB ILE 353
                               54.611 6.925 21.805 1.00 28.04
    ATOM 1104 CG2 ILE 353
                               53.329 6.111 22.065 1.00 23.68
                               54.269 8.251 21.119 1.00 27.33
    ATOM 1105 CG1 ILE 353
                               53.637 8.105 19.734 1.00 26.23
25
    ATOM 1106 CD1 ILE 353
                              55.631 5.943 23.901 1.00 30.88
    ATOM 1107 C ILE 353
    ATOM 1108 O ILE 353
                              54.880 5.597 24.814 1.00 31.22
    ATOM 1109 N PHE 354
                               56.710 5.240 23.549 1.00 29.86
    ATOM 1110 CA PHE 354
                               57.056 4.022 24.275 1.00 31.08
                               58.227 3.274 23.619 1.00 28.80
    ATOM 1111 CB PHE 354
30
                                57.799 2.322 22.523 1.00 28.80
    ATOM 1112 CG PHE 354
    ATOM 1113 CD1 PHE 354
                                57.330 2.804 21.292 1.00 30.96
    ATOM 1114 CD2 PHE 354
                                57.811 0.939 22.749 1.00 29.45
    ATOM 1115 CE1 PHE 354
                                56.864 1.909 20.281 1.00 27.12
    ATOM 1116 CE2 PHE 354
                                57.354 0.026 21.761 1.00 25.19
35
    ATOM 1117 CZ PHE 354
                               56.879 0.518 20.521 1.00 28.09
    ATOM 1118 C PHE 354
                               57.398 4.349 25.721 1.00 29.17
                               57.001 3.625 26.631 1.00 32.62
    ATOM 1119 O PHE 354
     ATOM 1120 N ASP 355
                               58.133 5.438 25.925 1.00 23.86
    ATOM 1121 CA ASP 355
                               58.508 5.873 27.262 1.00 25.34
40
     ATOM 1122 CB ASP 355
                               59.434 7.083 27.180 1.00 21.41
                                60.846 6.708 26.769 1.00 32.08
     ATOM 1123 CG ASP 355
     ATOM 1124 OD1 ASP 355
                                61.051 5.595 26.226 1.00 33.58
     ATOM 1125 OD2 ASP 355
                                61.756 7.534 26.970 1.00 33.20
                               57.254 6.211 28.062 1.00 27.86
45
     ATOM 1126 C ASP 355
                               57.167 5.916 29.252 1.00 32.42
     ATOM 1127 O ASP 355
     ATOM 1128 N LEU 356
                               56.276 6.821 27.401 1.00 26.84
     ATOM 1129 CA LEU 356
                                55.031 7.164 28.066 1.00 28.66
                                54.112 7.953 27.131 1.00 25.37
     ATOM 1130 CB LEU 356
                                52.787 8.427 27.742 1.00 27.61
    ATOM 1131 CG LEU 356
50
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ATOM 1132 CD1 LEU 356
                                53.056 9.452 28.842 1.00 25.43
                                51.924 9.057 26.667 1.00 27.49
     ATOM 1133 CD2 LEU 356
                               54.334 5.875 28.473 1.00 30.44
     ATOM 1134 C LEU 356
                               53.873 5.743 29.601 1.00 31.55
     ATOM 1135 O LEU 356
                               54.266 4.928 27.536 1.00 32.69
     ATOM 1136 N GLY 357
                                53.621 3.652 27.787 1.00 29.87
     ATOM 1137 CA GLY 357
     ATOM 1138 C GLY 357
                               54.239 2.884 28.939 1.00 33.12
     ATOM 1139 O GLY 357
                               53.524 2.268 29.732 1.00 29.41
     ATOM 1140 N MET 358
                               55.570 2.911 29.026 1.00 33.31
10
     ATOM 1141 CA MET 358
                                56.277 2.217 30.100 1.00 35.87
     ATOM 1142 CB MET 358
                                57.794 2.265 29.871 1.00 34.56
                                58.265 1.608 28.576 1.00 46.43
    ATOM 1143 CG MET 358
     ATOM 1144 SD MET 358
                                60.073 1.600 28.351 1.00 42.13
    ATOM 1145 CE MET 358
                                60.429 3.306 28.411 1.00 44.29
    ATOM 1146 C MET 358
                               55.948 2.884 31.434 1.00 33.26
15
     ATOM 1147 O MET 358
                               55.802 2.222 32.453 1.00 36.39
                               55.825 4.202 31.398 1.00 33.31
     ATOM 1148 N SER 359
    ATOM 1149 CA SER 359
                               55.533 4.998 32.580 1.00 34.39
                               55.859 6.463 32.303 1.00 30.84
     ATOM 1150 CB SER 359
    ATOM 1151 OG SER 359
                               55.487 7.265 33.404 1.00 47.14
20
                               54.094 4.897 33.072 1.00 36.43
     ATOM 1152 C SER 359
    ATOM 1153 O SER 359
                               53.833 5.073 34.260 1.00 35.46
     ATOM 1154 N LEU 360
                               53.165 4.617 32.156 1.00 36.74
                               51.750 4.519 32.493 1.00 35.44
    ATOM 1155 CA LEU 360
25
     ATOM 1156 CB LEU 360
                               50.889 4.817 31.263 1.00 34.16
                                50.896 6.263 30.751 1.00 34.59
     ATOM 1157 CG LEU 360
     ATOM 1158 CD1 LEU 360
                                50.031 6.353 29.513 1.00 33.53
     ATOM 1159 CD2 LEU 360
                                50.376 7.211 31.836 1.00 31.69
     ATOM 1160 C LEU 360
                               51.324 3.192 33.088 1.00 38.72
30
    ATOM 1161 O LEU 360
                               50.185 3.058 33.546 1.00 38.29
    ATOM 1162 N SER 361
                               52.227 2.214 33.080 1.00 40.96
    ATOM 1163 CA SER 361
                               51.938 0.897 33.636 1.00 45.67
                               53.131 -0.044 33.436 1.00 46.45
    ATOM 1164 CB SER 361
                               53.362 -0.296 32.061 1.00 51.81
    ATOM 1165 OG SER 361
                              51.628 1.004 35.124 1.00 44.49
    ATOM 1166 C SER 361
35
    ATOM 1167 O SER 361
                               50.724 0.337 35.630 1.00 46.67
    ATOM 1168 N SER 362
                               52.385 1.858 35.809 1.00 41.44
                               52.231 2.081 37.245 1.00 42.13
    ATOM 1169 CA SER 362
    ATOM 1170 CB SER 362
                               53.431 2.876 37.779 1.00 42.61
                               54.647 2.215 37.492 1.00 51.87
40
    ATOM 1171 OG SER 362
                              50.951 2.832 37.610 1.00 38.41
    ATOM 1172 C SER 362
                               50.444 2.700 38.722 1.00 38.01
     ATOM 1173 O SER 362
    ATOM 1174 N PHE 363
                               50.443 3.631 36.672 1.00 34.55
    ATOM 1175 CA PHE 363
                               49.232 4.404 36.906 1.00 32.96
45
    ATOM 1176 CB PHE 363
                               49.109 5.518 35.859 1.00 31.99
                               50.093 6.659 36.058 1.00 29.97
    ATOM 1177 CG PHE 363
    ATOM 1178 CD1 PHE 363
                                49.667 7.872 36.594 1.00 30.61
                                51.445 6.501 35.731 1.00 32.02
     ATOM 1179 CD2 PHE 363
    ATOM 1180 CE1 PHE 363
                                50.579 8.940 36.803 1.00 33.67
                                52.376 7.552 35.934 1.00 30.91
50
    ATOM 1181 CE2 PHE 363
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ATOM 1182 CZ PHE 363
                               51.938 8.777 36.473 1.00 29.33
                               47.973 3.554 36.916 1.00 30.52
     ATOM 1183 C PHE 363
     ATOM 1184 O PHE 363
                               46.971 3.947 37.491 1.00 32.19
     ATOM 1185 N ASN 364
                               48.036 2.384 36.283 1.00 33.51
     ATOM 1186 CA ASN 364
                                46.894 1.471 36.216 1.00 38.03
     ATOM 1187 CB ASN 364
                                46.754 0.711 37.539 1.00 42.32
                                47,824 -0.361 37.713 1.00 53.11
     ATOM 1188 CG ASN 364
     ATOM 1189 OD1 ASN 364
                                47.815 -1.370 37.012 1.00 59.51
     ATOM 1190 ND2 ASN 364
                                48.751 -0.138 38.639 1.00 55.95
                               45.574 2.161 35.871 1.00 31.89
     ATOM 1191 C ASN 364
10
                               44.587 2.027 36.588 1.00 30.28
     ATOM 1192 O ASN 364
    ATOM 1193 N LEU 365
                               45.561 2.883 34.751 1.00 27.62
     ATOM 1194 CA LEU 365
                               44.365 3.606 34.317 1.00 29.36
     ATOM 1195 CB LEU 365
                               44.738 4.627 33.240 1.00 27.54
    ATOM 1196 CG LEU 365
                                45.826 5.659 33.576 1.00 38.91
15
                                46.115 6.499 32.338 1.00 34.47
     ATOM 1197 CD1 LEU 365
    ATOM 1198 CD2 LEU 365
                                45.394 6.546 34.743 1.00 34.24
     ATOM 1199 C LEU 365
                               43.264 2.691 33.774 1.00 26.23
                               43.546 1.648 33.197 1.00 27.06
     ATOM 1200 O LEU 365
                              42.011 3.074 33.991 1.00 25.23
     ATOM 1201 N ASP 366
20
                              40.892 2.307 33.462 1.00 26.07
    ATOM 1202 CA ASP 366
                               39.832 2.008 34.538 1.00 29.68
    ATOM 1203 CB ASP 366
                               39.337 3.253 35.261 1.00 35.74
     ATOM 1204 CG ASP 366
     ATOM 1205 OD1 ASP 366
                                39.438 4.371 34.717 1.00 36.78
    ATOM 1206 OD2 ASP 366
                                38.803 3.100 36.378 1.00 41.23
25
    ATOM 1207 C ASP 366
                              40.274 3.100 32.305 1.00 27.70
                               40.748 4.191 31.975 1.00 31.94
     ATOM 1208 O ASP 366
                               39.223 2.564 31.693 1.00 29.18
     ATOM 1209 N ASP 367
                               38.594 3.233 30.560 1.00 32.72
     ATOM 1210 CA ASP 367
    ATOM 1211 CB ASP 367
                               37.428 2.395 30.018 1.00 38.04
30
     ATOM 1212 CG ASP 367
                               37.855 0.995 29.606 1.00 42.43
    ATOM 1213 OD1 ASP 367
                                38.913 0.852 28.956 1.00 35.95
    ATOM 1214 OD2 ASP 367
                                37.115 0.034 29.917 1.00 51.42
                              38.093 4.631 30.881 1.00 33.71
    ATOM 1215 C ASP 367
                               38.059 5.506 30.013 1.00 38.30
3.5
    ATOM 1216 O ASP 367
                               37.705 4.852 32.132 1.00 31.06
     ATOM 1217 N THR 368
    ATOM 1218 CA THR 368
                                37.199 6.155 32.543 1.00 26.28
    ATOM 1219 CB THR 368
                               36.537 6.066 33.922 1.00 27.30
     ATOM 1220 OG1 THR 368
                                35.461 5.127 33.861 1.00 33.42
40
    ATOM 1221 CG2 THR 368
                                36.003 7.423 34.355 1.00 25.16
     ATOM 1222 C THR 368
                               38.303 7.194 32.593 1.00 21.13
     ATOM 1223 O THR 368
                               38.133 8.314 32.104 1.00 23.17
     ATOM 1224 N GLU 369
                               39.431 6.816 33.179 1.00 21.32
    ATOM 1225 CA GLU 369
                                40.565 7.720 33.317 1.00 28.00
                                41.582 7.107 34.277 1.00 32.79
    ATOM 1226 CB GLU 369
45
    ATOM 1227 CG GLU 369
                                40.944 6.804 35.619 1.00 36.29
                                41.834 6.026 36.546 1.00 41.03
     ATOM 1228 CD GLU 369
                                42.361 4.967 36.123 1.00 42.05
     ATOM 1229 OE1 GLU 369
                                41.986 6.458 37.705 1.00 42.03
    ATOM 1230 OE2 GLU 369
                               41.201 8.047 31.970 1.00 25.57
50
    ATOM 1231 C GLU 369
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41.626 9.175 31.741 1.00 20.56
    ATOM 1232 O GLU 369
                               41.249 7.055 31.080 1.00 25.39
    ATOM 1233 N VAL 370
                                41.794 7.278 29.745 1.00 25.99
    ATOM 1234 CA VAL 370
                                42.005 5.936 28.977 1.00 26.15
    ATOM 1235 CB VAL 370
                                42.450 6.216 27.539 1.00 27.65
    ATOM 1236 CG1 VAL 370
    ATOM 1237 CG2 VAL 370
                                43.056 5.086 29.685 1.00 17.70
                               40.814 8.164 28.966 1.00 26.49
    ATOM 1238 C VAL 370
                               41.226 9.038 28.202 1.00 28.16
    ATOM 1239 O VAL 370
                               39.514 7.950 29.184 1.00 21.01
    ATOM 1240 N ALA 371
                                38.486 8.730 28.510 1.00 19.57
    ATOM 1241 CA ALA 371
10
                                37.116 8.136 28.783 1.00 18.62
    ATOM 1242 CB ALA 371
                               38.512 10.191 28.947 1.00 23.48
    ATOM 1243 C ALA 371
                               38.500 11.103 28.111 1.00 32.67
    ATOM 1244 O ALA 371
                               38.540 10.414 30.256 1.00 22.89
    ATOM 1245 N LEU 372
                               38.560 11.772 30.806 1.00 23.28
    ATOM 1246 CA LEU 372
15
                                38.517 11.709 32.343 1.00 27.76
    ATOM 1247 CB LEU 372
    ATOM 1248 CG LEU 372
                                37.155 11.306 32.924 1.00 21.18
                                37,289 10,891 34,381 1,00 27,64
    ATOM 1249 CD1 LEU 372
    ATOM 1250 CD2 LEU 372
                                36.197 12.480 32.763 1.00 20.90
                               39.804 12.505 30.357 1.00 21.34
    ATOM 1251 C LEU 372
20
                               39.779 13.708 30.086 1.00 23.16
    ATOM 1252 O LEU 372
                               40.896 11.761 30.276 1.00 24.42
    ATOM 1253 N LEU 373
                                42.177 12.302 29.855 1.00 23.78
    ATOM 1254 CA LEU 373
                                43.222 11.205 30.007 1.00 22.18
    ATOM 1255 CB LEU 373
    ATOM 1256 CG LEU 373
                                44.724 11.456 30.036 1.00 31.52
25
    ATOM 1257 CD1 LEU 373
                                45.099 12.565 31.001 1.00 31.93
                                45.382 10.152 30.460 1.00 30.24
    ATOM 1258 CD2 LEU 373
                               42.025 12.757 28.399 1.00 25.69
    ATOM 1259 C LEU 373
                               42.469 13.842 28.025 1.00 30.13
    ATOM 1260 O LEU 373
                               41.370 11.934 27.587 1.00 26.24
    ATOM 1261 N GLN 374
30
                                41.151 12.269 26.184 1.00 21.60
    ATOM 1262 CA GLN 374
                                40.501 11.091 25.444 1.00 24.57
    ATOM 1263 CB GLN 374
                                41.428 9.900 25.234 1.00 21.02
    ATOM 1264 CG GLN 374
                                40.762 8.744 24.501 1.00 22.86
    ATOM 1265 CD GLN 374
                                41.407 7.754 24.174 1.00 24.07
    ATOM 1266 OE1 GLN 374
35
                                39,466 8.865 24.249 1.00 25.59
    ATOM 1267 NE2 GLN 374
                               40,267 13,498 26.070 1.00 20.66
    ATOM 1268 C GLN 374
                               40.518 14.366 25.242 1.00 24.47
    ATOM 1269 O GLN 374
                               39.237 13.579 26.902 1.00 16.26
    ATOM 1270 N ALA 375
     ATOM 1271 CA ALA 375
                                38.337 14.727 26.870 1.00 17.16
40
                                37.156 14.491 27.803 1.00 19.53
    ATOM 1272 CB ALA 375
    ATOM 1273 C ALA 375
                               39.056 16.024 27.252 1.00 25.13
                               38.722 17.100 26.750 1.00 23.81
     ATOM 1274 O ALA 375
                               40.036 15.926 28.156 1.00 24.57
     ATOM 1275 N VAL 376
                                40.796 17.101 28.568 1.00 25.80
     ATOM 1276 CA VAL 376
45
                                41.711 16.792 29.814 1.00 26.48
     ATOM 1277 CB VAL 376
                                42.625 17.971 30.102 1.00 23.20
     ATOM 1278 CG1 VAL 376
     ATOM 1279 CG2 VAL 376
                                40.845 16.521 31.044 1.00 19.08
                               41.653 17.580 27.396 1.00 25.69
     ATOM 1280 C VAL 376
     ATOM 1281 O VAL 376
                               41.775 18.780 27.151 1.00 27.87
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	ATOM	1282 N LEU 377	42.249 16.637 26.666 1.00 23.09
	ATOM	1283 CA LEU 377	43.071 16.982 25.513 1.00 22.86
	ATOM	1284 CB LEU 377	43.748 15.730 24.962 1.00 18.50
	ATOM	1285 CG LEU 377	44.814 15.096 25.867 1.00 22.65
5	ATOM	1286 CD1 LEU 377	45.144 13.708 25.374 1.00 16.70
	ATOM	1287 CD2 LEU 377	46.070 15.987 25.901 1.00 19.58
	ATOM	1288 C LEU 377	42.197 17.634 24.430 1.00 26.14
	ATOM	1289 O LEU 377	42.579 18.638 23.830 1.00 20.62
	ATOM	1290 N LEU 378	41.016 17.057 24.208 1.00 28.99
10	ATOM	1291 CA LEU 378	40.076 17.578 23.218 1.00 28.87
	ATOM	1292 CB LEU 378	38.814 16.710 23.182 1.00 26.89
	ATOM	1293 CG LEU 378	37.637 17.167 22.311 1.00 28.83
	ATOM	1294 CD1 LEU 378	38.053 17.273 20.840 1.00 27.97
	ATOM	1295 CD2 LEU 378	36.496 16.175 22.478 1.00 27.69
15	ATOM	1296 C LEU 378	39.693 19.025 23.504 1.00 31.09
	ATOM	1297 O LEU 378	39.812 19.883 22.629 1.00 31.77
	ATOM	1298 N MET 379	39.247 19.297 24.729 1.00 31.44
	ATOM	1299 CA MET 379	38.841 20.649 25.104 1.00 32.62
	ATOM	1300 CB MET 379	37.876 20.603 26.293 1.00 31.45
20	ATOM	1301 CG MET 379	36.586 19.855 26.010 1.00 38.75
	ATOM	1302 SD MET 379	35.646 20.541 24.601 1.00 41.27
	ATOM	1303 CE MET 379	34.231 19.443 24.609 1.00 35.68
	ATOM	1304 C MET 379	39.980 21.613 25.421 1.00 33.72
	ATOM	1305 O MET 379	39.940 22.297 26.446 1.00 36.29
25	ATOM	1306 N SER 380	40.981 21.676 24.543 1.00 34.49
	ATOM	1307 CA SER 380	42.116 22.585 24.721 1.00 33.97
	ATOM	1308 CB SER 380	43.371 22.025 24.061 1.00 31.24
	ATOM	1309 OG SER 380	43.771 20.814 24.674 1.00 39.42
	ATOM	1310 C SER 380	41.772 23.926 24.088 1.00 39.69
30	ATOM	1311 O SER 380	41.787 24.069 22.864 1.00 44.64
	ATOM	1312 N SER 381	41.472 24.907 24.927 1.00 41.04
	ATOM	1313 CA SER 381	41.090 26.234 24.462 1.00 44.91
	ATOM	1314 CB SER 381	40.406 27.004 25.594 1.00 44.50
2.5	ATOM	1315 OG SER 381	41.294 27.177 26.678 1.00 45.42
35	ATOM	1316 C SER 381	42.231 27.084 23.921 1.00 44.59 42.012 28.227 23.516 1.00 49.32
	ATOM	1317 O SER 381 1318 N ASP 382	43.440 26.541 23.896 1.00 43.75
	ATOM		44.571 27.315 23.407 1.00 43.73
	ATOM	1319 CA ASP 382 1320 CB ASP 382	45.817 27.047 24.257 1.00 48.39
40	ATOM	1320 CB ASP 382 1321 CG ASP 382	46.319 25.632 24.113 1.00 53.23
40	ATOM ATOM	1321 CG ASP 382 1322 OD1 ASP 382	45.590 24.702 24.517 1.00 56.97
	ATOM	1322 OD1 ASP 382 1323 OD2 ASP 382	47.440 25.449 23.584 1.00 58.91
	ATOM	1324 C ASP 382	44.900 27.026 21.955 1.00 41.09
	ATOM	1325 O ASP 382	45.912 27.502 21.446 1.00 40.93
45	ATOM	1325 O ASP 382 1326 N ARG 383	44.068 26.236 21.287 1.00 42.63
ر4	ATOM	1326 N ARG 383	44.316 25.937 19.876 1.00 42.03
	ATOM	1327 CA ARG 383	43.289 24.935 19.331 1.00 42.31
	ATOM	1329 CG ARG 383	43.174 23.619 20.095 1.00 40.83
	ATOM		44.478 22.835 20.139 1.00 38.09
50	ATOM		44.271 21.542 20.787 1.00 37.33
55	1110111	112 /110 505	

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ATOM 1332 CZ ARG 383
                                45.235 20.690 21.115 1.00 38.35
                                 46.505 20.972 20.850 1.00 33.70
    ATOM 1333 NH1 ARG 383
                                 44.922 19.545 21.704 1.00 35.46
     ATOM 1334 NH2 ARG 383
    ATOM 1335 C ARG 383
                               44.166 27.256 19.127 1.00 44.96
    ATOM 1336 O ARG 383
                               43.214 28.006 19.361 1.00 45.60
                               45.112 27.574 18.230 1.00 45.33
    ATOM 1337 N PRO 384
                                46.330 26.852 17.836 1.00 46.85
    ATOM 1338 CD PRO 384
    ATOM 1339 CA PRO 384
                                45.024 28.830 17.484 1.00 47.37
    ATOM 1340 CB PRO 384
                                46.323 28.823 16.672 1.00 46.90
                                47.257 27.998 17.552 1.00 46.41
    ATOM 1341 CG PRO 384
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    ATOM 1342 C PRO 384
                               43.788 28.910 16.590 1.00 48.29
    ATOM 1343 O PRO 384
                               43.394 27.927 15.960 1.00 48.34
    ATOM 1344 N GLY 385
                               43.176 30.090 16.552 1.00 49.88
                                42.013 30.290 15.712 1.00 50.35
    ATOM 1345 CA GLY 385
                               40.669 29.958 16.324 1.00 50.70
    ATOM 1346 C GLY 385
15
                               39.639 30.201 15.697 1.00 53.48
     ATOM 1347 O GLY 385
                               40.663 29.404 17.529 1.00 49.04
    ATOM 1348 N LEU 386
                                39.405 29.057 18.182 1.00 50.53
    ATOM 1349 CA LEU 386
    ATOM 1350 CB LEU 386
                                39.655 28.433 19.558 1.00 45.17
    ATOM 1351 CG LEU 386
                                40.245 27.019 19.544 1.00 48.26
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    ATOM 1352 CD1 LEU 386
                                40.502 26.564 20.970 1.00 41.68
                                39.285 26.065 18.836 1.00 38.40
    ATOM 1353 CD2 LEU 386
                               38.495 30.268 18.319 1.00 52.13
    ATOM 1354 C LEU 386
    ATOM 1355 O LEU 386
                               38.955 31.395 18.476 1.00 53.67
25
    ATOM 1356 N ALA 387
                               37.193 30.020 18.261 1.00 53.42
                                36.225 31.093 18.354 1.00 56.01
    ATOM 1357 CA ALA 387
    ATOM 1358 CB ALA 387
                                35.221 30.976 17.202 1.00 56.47
    ATOM 1359 C ALA 387
                               35,482 31.144 19.681 1.00 55.52
                               35.491 32.171 20.358 1.00 53.75
    ATOM 1360 O ALA 387
                               34.854 30.038 20.065 1.00 56.03
    ATOM 1361 N CYS 388
30
                                34.072 30.036 21.312 1.00 59.57
     ATOM 1362 CA CYS 388
                                32.724 29.351 21.089 1.00 59.23
     ATOM 1363 CB CYS 388
     ATOM 1364 SG CYS 388
                                31.314 30.363 21.641 1.00 58.64
                               34.846 29.289 22.398 1.00 62.18
     ATOM 1365 C CYS 388
                               34.458 28.190 22.790 1.00 67.88
     ATOM 1366 O CYS 388
35
                               35.955 29.950 22.760 1.00 60.78
    ATOM 1367 N VAL 389
                                37.005 29.583 23.713 1.00 57.70
    ATOM 1368 CA VAL 389
     ATOM 1369 CB VAL 389
                                38.202 30.580 23.565 1.00 57.09
     ATOM 1370 CG1 VAL 389
                                39.351 30.194 24.494 1.00 59.03
    ATOM 1371 CG2 VAL 389
                                38.671 30.618 22.124 1.00 53.98
40
                               36.661 29.515 25.195 1.00 57.77
     ATOM 1372 C VAL 389
     ATOM 1373 O VAL 389
                               36.943 28.513 25.851 1.00 60.94
                               36.102 30.594 25.732 1.00 52.68
     ATOM 1374 N GLU 390
     ATOM 1375 CA GLU 390
                                35.738 30.636 27.138 1.00 48.41
                                35.001 31.928 27.451 1.00 45.19
45
     ATOM 1376 CB GLU 390
     ATOM 1377 C GLU 390
                               34.868 29.439 27.459 1.00 47.63
     ATOM 1378 O GLU 390
                               34.986 28.837 28.529 1.00 51.95
                               34.002 29.082 26.517 1.00 47.11
     ATOM 1379 N ARG 391
     ATOM 1380 CA ARG 391
                                33.099 27.950 26.699 1.00 51.64
                                32.050 27.930 25.588 1.00 54.22
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     ATOM 1381 CB ARG 391
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ATOM 1382 CG ARG 391
                                30.830 27.094 25.915 1.00 64.20
     ATOM 1383 CD ARG 391
                                29.867 27.074 24.748 1.00 73.80
     ATOM 1384 NE ARG 391
                                28.533 26.622 25.128 1.00 79.76
     ATOM 1385 CZ ARG 391
                                27.714 27.298 25.929 1.00 84.27
     ATOM 1386 NH1 ARG 391
                                 28.090 28.465 26.439 1.00 85.28
                                 26.515 26.809 26.217 1.00 86.84
     ATOM 1387 NH2 ARG 391
                               33.890 26.644 26.684 1.00 48.18
     ATOM 1388 C ARG 391
                               33.504 25.671 27.330 1.00 49.57
     ATOM 1389 O ARG 391
                              34.987 26.625 25.936 1.00 45.01
     ATOM 1390 N ILE 392
                               35.835 25.440 25.858 1.00 48.77
     ATOM 1391 CA ILE 392
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                               36.854 25.565 24.692 1.00 46.45
     ATOM 1392 CB ILE 392
                               37.798 24.370 24.679 1.00 42.35
     ATOM 1393 CG2 ILE 392
                               36.086 25.664 23.367 1.00 49.69
     ATOM 1394 CG1 ILE 392
                                36.950 25.897 22.136 1.00 51.09
     ATOM 1395 CD1 ILE 392
                              36.570 25.246 27.192 1.00 50.90
     ATOM 1396 C ILE 392
15
                              36,731 24.118 27.657 1.00 52.21
     ATOM 1397 O ILE 392
                               36.999 26.346 27.811 1.00 50.43
     ATOM 1398 N GLU 393
                                37.673 26.267 29.101 1.00 50.30
     ATOM 1399 CA GLU 393
                                38.202 27.638 29.531 1.00 53.97
     ATOM 1400 CB GLU 393
                                39.322 28.168 28.658 1.00 62.18
     ATOM 1401 CG GLU 393
20
                                39.911 29.478 29.168 1.00 67.69
     ATOM 1402 CD GLU 393
                                40.869 29.977 28.537 1.00 66.42
     ATOM 1403 OE1 GLU 393
     ATOM 1404 OE2 GLU 393
                                39.423 30.009 30.191 1.00 70.64
                               36.686 25.765 30.145 1.00 49.31
     ATOM 1405 C GLU 393
                               37.018 24.923 30.980 1.00 49.53
25
     ATOM 1406 O GLU 393
                               35.468 26.286 30.090 1.00 46.07
     ATOM 1407 N LYS 394
                                34.428 25.893 31.022 1.00 45.76
     ATOM 1408 CA LYS 394
                                33.147 26.666 30.727 1.00 43.85
     ATOM 1409 CB LYS 394
                               34.188 24.391 30.909 1.00 46.69
     ATOM 1410 C LYS 394
                               33.982 23.699 31.911 1.00 49.13
30
     ATOM 1411 O LYS 394
                               34.223 23.887 29.679 1.00 46.57
     ATOM 1412 N TYR 395
     ATOM 1413 CA TYR 395
                                34.014 22.467 29.427 1.00 43.33
     ATOM 1414 CB TYR 395.
                                33.818 22.211 27.929 1.00 48.44
     ATOM 1415 CG TYR 395
                                32.493 22.710 27.335 1.00 53.83
                                32.302 22.727 25.947 1.00 56.43
35
     ATOM 1416 CD1 TYR 395
                                31.078 23.148 25.374 1.00 59.73
     ATOM 1417 CE1 TYR 395
     ATOM 1418 CD2 TYR 395
                                 31.434 23.132 28.153 1.00 56.47
                                30,198 23.559 27.592 1.00 62.60
     ATOM 1419 CE2 TYR 395
     ATOM 1420 CZ TYR 395
                                30.037 23.562 26.200 1.00 63.18
     ATOM 1421 OH TYR 395
                                28.834 23.962 25.635 1.00 64.46
40
                               35.189 21.635 29.938 1.00 37.30
     ATOM 1422 C TYR 395
                               34.993 20.599 30.564 1.00 34.10
     ATOM 1423 O TYR 395
     ATOM 1424 N GLN 396
                               36.408 22.091 29.671 1.00 31.92
                                37.584 21.363 30.120 1.00 34.81
     ATOM 1425 CA GLN 396
                                38.861 21.987 29.560 1.00 32.64
     ATOM 1426 CB GLN 396
45
     ATOM 1427 CG GLN 396
                                40.114 21.183 29.882 1.00 29.57
                                41.370 21.827 29.352 1.00 29.46
     ATOM 1428 CD GLN 396
     ATOM 1429 OE1 GLN 396
                                41.648 22.982 29.649 1.00 34.65
                                42.139 21.088 28.570 1.00 27.21
     ATOM 1430 NE2 GLN 396
                               37.647 21.342 31.647 1.00 37.13
     ATOM 1431 C GLN 396
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37.939 20.302 32.236 1.00 37.36
    ATOM 1432 O GLN 396
                               37.371 22.484 32.284 1.00 38.61
     ATOM 1433 N ASP 397
                                37.393 22.555 33.742 1.00 40.37
    ATOM 1434 CA ASP 397
     ATOM 1435 CB ASP 397
                                37.099 23.973 34.240 1.00 40.51
    ATOM 1436 CG ASP 397
                                38.130 24.974 33.772 1.00 43.77
                                39.330 24.632 33.775 1.00 46.50
     ATOM 1437 OD1 ASP 397
    ATOM 1438 OD2 ASP 397
                                37.750 26.109 33.422 1.00 51.34
     ATOM 1439 C ASP 397
                               36.352 21.601 34.295 1.00 38.62
     ATOM 1440 O ASP 397
                               36.515 21.034 35.372 1.00 39.20
    ATOM 1441 N SER 398
                               35.282 21.423 33.540 1.00 37.84
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    ATOM 1442 CA SER 398
                               34.221 20.524 33.942 1.00 37.80
    ATOM 1443 CB SER 398
                                33.039 20.669 32.984 1.00 34.28
    ATOM 1444 OG SER 398
                                31.981 19.815 33.360 1.00 46.60
                               34.752 19.082 33.939 1.00 38.41
     ATOM 1445 C SER 398
     ATOM 1446 O SER 398
                               34.372 18.274 34.787 1.00 39.98
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     ATOM 1447 N PHE 399
                               35,630 18,772 32,987 1.00 34.82
                                36.213 17.433 32.885 1.00 35.96
    ATOM 1448 CA PHE 399
    ATOM 1449 CB PHE 399
                                36.809 17.181 31.493 1.00 35.75
     ATOM 1450 CG PHE 399
                                35.775 16.936 30.419 1.00 39.30
20
    ATOM 1451 CD1 PHE 399
                                35.640 17.826 29.344 1.00 39.86
                                34.936 15.819 30.487 1.00 36.81
     ATOM 1452 CD2 PHE 399
     ATOM 1453 CE1 PHE 399
                                34.674 17.607 28.330 1.00 41.25
                                33.962 15.577 29.488 1.00 43.61
     ATOM 1454 CE2 PHE 399
     ATOM 1455 CZ PHE 399
                               33.829 16.480 28.402 1.00 40.34
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     ATOM 1456 C PHE 399
                               37.306 17.217 33.921 1.00 33.48
     ATOM 1457 O PHE 399
                               37.406 16.139 34.512 1.00 26.86
     ATOM 1458 N LEU 400
                               38.132 18.239 34.118 1.00 31.47
    ATOM 1459 CA LEU 400
                                39.213 18.162 35.086 1.00 37.41
     ATOM 1460 CB LEU 400
                                40.051 19.441 35.038 1.00 34.24
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     ATOM 1461 CG LEU 400
                                40.934 19.574 33.788 1.00 35.10
     ATOM 1462 CD1 LEU 400
                                41.469 20.991 33.651 1.00 26.60
     ATOM 1463 CD2 LEU 400
                                42.077 18.569 33.884 1.00 29.44
     ATOM 1464 C LEU 400
                               38.666 17.931 36.491 1.00 38.84
     ATOM 1465 O LEU 400
                               39.137 17.049 37.205 1.00 40.38
     ATOM 1466 N LEU 401
                               37.654 18.703 36.870 1.00 42.79
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     ATOM 1467 CA LEU 401
                                37.056 18.584 38.197 1.00 43.48
                                35.997 19.675 38.406 1.00 44.73
     ATOM 1468 CB LEU 401
                                35.322 19.737 39.779 1.00 51.39
     ATOM 1469 CG LEU 401
                                36.359 20.002 40.866 1.00 50.11
     ATOM 1470 CD1 LEU 401
                                34.273 20,834 39.778 1.00 49.30
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     ATOM 1471 CD2 LEU 401
                               36.433 17.215 38.409 1.00 41.62
     ATOM 1472 C LEU 401
     ATOM 1473 O LEU 401
                               36.563 16.622 39.482 1.00 45.14
                               35.744 16.712 37.389 1.00 37.92
     ATOM 1474 N ALA 402
                                35.115 15.402 37.484 1.00 29.90
     ATOM 1475 CA ALA 402
     ATOM 1476 CB ALA 402
                                34.196 15.187 36.297 1.00 30.70
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     ATOM 1477 C ALA 402
                               36.203 14.336 37.508 1.00 28.88
     ATOM 1478 O ALA 402
                               36.083 13.322 38.188 1.00 32.14
                               37.274 14.588 36.764 1.00 31.07
     ATOM 1479 N PHE 403
     ATOM 1480 CA PHE 403
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                                39.396 14.178 35.605 1.00 27.03
     ATOM 1481 CB PHE 403
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ATOM 1482 CG PHE 403
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     ATOM 1483 CD1 PHE 403
                                 41.362 13.509 34.149 1.00 25.55
     ATOM 1484 CD2 PHE 403
                                 40.475 11.841 35.664 1.00 19.75
     ATOM 1485 CE1 PHE 403
                                42,331 12.588 33.679 1.00 27.90
     ATOM 1486 CE2 PHE 403
                                41.441 10.899 35.206 1.00 22.56
     ATOM 1487 CZ PHE 403
                                42.371 11.273 34.210 1.00 22.24
                               39.081 13.523 38.023 1.00 28.82
     ATOM 1488 C PHE 403
     ATOM 1489 O PHE 403
                               39.313 12.413 38.495 1.00 26.00
     ATOM 1490 N GLU 404
                               39.405 14.652 38.652 1.00 30.25
                                40.039 14.627 39.966 1.00 34.03
     ATOM 1491 CA GLU 404
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     ATOM 1492 CB GLU 404
                                40.264 16.046 40.497 1.00 39.45
                                40.987 16.076 41.839 1.00 47.68
     ATOM 1493 CG GLU 404
     ATOM 1494 CD GLU 404
                                41.062 17.465 42.446 1.00 54.02
     ATOM 1495 OE1 GLU 404
                                 41.607 18.380 41.796 1.00 57.27
                                 40.573 17.638 43.585 1.00 63.85
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     ATOM 1496 OE2 GLU 404
     ATOM 1497 C GLU 404
                               39.164 13.860 40.960 1.00 36.01
     ATOM 1498 O GLU 404
                                39.661 12.997 41.701 1.00 38.64
     ATOM 1499 N HIS 405
                               37.870 14.168 40.975 1.00 29.56
     ATOM 1500 CA HIS 405
                               36.949 13.508 41.892 1.00 31.69
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     ATOM 1501 CB HIS 405
                               35.534 14.077 41.757 1.00 33.75
     ATOM 1502 CG HIS 405
                               35.401 15.498 42.213 1.00 34.75
     ATOM 1503 CD2 HIS 405
                                36.308 16.361 42.730 1.00 34.58
     ATOM 1504 ND1 HIS 405
                                34.207 16.187 42.146 1.00 32.43
     ATOM 1505 CE1 HIS 405
                                34.385 17.414 42.598 1.00 36.15
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     ATOM 1506 NE2 HIS 405
                                35.650 17.549 42.960 1.00 39.84
     ATOM 1507 C HIS 405
                               36.904 12.013 41.673 1.00 34.21
     ATOM 1508 O HIS 405
                               36.700 11.247 42.624 1.00 37.06
     ATOM 1509 N TYR 406
                               37.081 11.594 40.419 1.00 30.83
     ATOM 1510 CA TYR 406
                                37.059 10.173 40.093 1.00 28.85
     ATOM 1511 CB TYR 406
                                37.018 9.959 38.575 1.00 31.48
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     ATOM 1512 CG TYR 406
                                36.879 8.490 38.181 1.00 23.49
                                35.683 7.798 38.397 1.00 19.42
     ATOM 1513 CD1°TYR 406
     ATOM 1514 CE1 TYR 406
                                35.556 6.427 38.059 1.00 23.80
     ATOM 1515 CD2 TYR 406
                                37.950 7.794 37.624 1.00 21.81
35
    ATOM 1516 CE2 TYR 406
                                37.838 6.421 37.278 1.00 24.64
    ATOM 1517 CZ TYR 406
                                36.639 5.753 37.503 1.00 21.56
    ATOM 1518 OH TYR 406
                                36.537 4.404 37.186 1.00 24.96
     ATOM 1519 C TYR 406
                               38.318 9.526 40.638 1.00 24.24
    ATOM 1520 O TYR 406
                               38.308 8.375 41.050 1.00 27.08
40
    ATOM 1521 N ILE 407
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    ATOM 1522 CA ILE 407
                               40.688 9.799 41.105 1.00 33.75
    ATOM 1523 CB ILE 407
                               41.815 10.822 40.796 1.00 34.23
    ATOM 1524 CG2 ILE 407
                               43.121 10.400 41.435 1.00 32.46
    ATOM 1525 CG1 ILE 407
                               41.959 10.972 39.275 1.00 43.30
                               42.267 9.677 38.523 1.00 40.40
45
    ATOM 1526 CD1 ILE 407
    ATOM 1527 C ILE 407
                              40.620 9.556 42.613 1.00 39.03
    ATOM 1528 O ILE 407
                              41.192 8.583 43.107 1.00 35.18
    ATOM 1529 N ASN 408
                               39.916 10.440 43.335 1.00 37.25
    ATOM 1530 CA ASN 408
                               39.778 10.292 44.777 1.00 37.01
50
                                39.099 11.514 45.400 1.00 32.27
    ATOM 1531 CB ASN 408
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	ATOM	1532 CG ASN 408 39.887 12.790 45.187 1.00 33.56
	ATOM	1533 OD1 ASN 408 41.118 12.785 45.225 1.00 31.99
	ATOM	1534 ND2 ASN 408 39.182 13.903 44.996 1.00 31.23
	ATOM	1535 C ASN 408 38.961 9.046 45.055 1.00 38.14
5	ATOM	1536 O ASN 408 39.303 8.243 45.920 1.00 42.16
3		
	ATOM	
	ATOM ATOM	1538 CA TYR 409 37.002 7.733 44.412 1.00 35.91 1539 CB TYR 409 35.929 7.804 43.323 1.00 34.41
10	ATOM	
10	ATOM ATOM	1541 CD1 TYR 409 34.266 5.982 43.980 1.00 41.34 1542 CE1 TYR 409 33.600 4.745 43.741 1.00 47.16
	ATOM	
		1543 CD2 TYR 409 35.461 5.752 41.907 1.00 46.20 1544 CE2 TYR 409 34.814 4.518 41.651 1.00 50.74
	ATOM	
1.5	ATOM	1545 CZ TYR 409 33.891 4.023 42.573 1.00 50.88
15	ATOM	1546 OH TYR 409 33.262 2.816 42.302 1.00 53.14
	ATOM	1547 C TYR 409 37.827 6.459 44.240 1.00 38.16
	ATOM	1548 O TYR 409 37.806 5.561 45.082 1.00 41.83
	ATOM	1549 N ARG 410 38.551 6.399 43.125 1.00 42.25
20	ATOM	1550 CA ARG 410 39.410 5.272 42.765 1.00 42.83
20	ATOM ATOM	1551 CB ARG 410 40.029 5.540 41.392 1.00 36.83 1552 CG ARG 410 39.055 5.397 40.249 1.00 34.32
	ATOM	1553 CD ARG 410 39.033 3.397 40.249 1.00 34.32
	ATOM	1554 NE ARG 410 40.420 3.787 39.013 1.00 38.64
	ATOM	1555 CZ ARG 410 40.832 2.625 38.517 1.00 35.73
25	ATOM	1556 NH1 ARG 410 40.068 1.548 38.617 1.00 33.17
23	ATOM	1557 NH2 ARG 410 42.006 2.544 37.916 1.00 32.70
	ATOM	1558 C ARG 410 40.520 5.039 43.780 1.00 46.67
	ATOM	1559 O ARG 410 40.900 3.901 44.053 1.00 41.78
	ATOM	1560 N LYS 411 41.026 6.140 44.325 1.00 52.99
30	ATOM	1561 CA LYS 411 42.109 6.141 45.298 1.00 58.32
	ATOM	1562 CB LYS 411 41.565 5.956 46.731 1.00 64.99
	ATOM	1563 CG LYS 411 40.660 4.763 46.977 1.00 70.48
	ATOM	1564 CD LYS 411 40.034 4.866 48.364 1.00 77.18
	ATOM	1565 CE LYS 411 39.053 3.732 48.625 1.00 84.30
35	ATOM	1566 NZ LYS 411 38.392 3.865 49.958 1.00 86.48
	ATOM	1567 C LYS 411 43.238 5.163 45.000 1.00 56.66
	ATOM	1568 O LYS 411 43.329 4.075 45.575 1.00 55.47
	ATOM	1569 N HIS 412 44.091 5.582 44.070 1.00 54.67
	ATOM	1570 CA HIS 412 45.266 4.823 43.657 1.00 48.67
40	ATOM	1571 CB HIS 412 45.878 5.442 42.393 1.00 43.14
	ATOM	1572 CG HIS 412 45.073 5.218 41.156 1.00 41.36
	ATOM	1573 CD2 HIS 412 44.084 5.952 40.584 1.00 35.44
	ATOM	1574 ND1 HIS 412 45.220 4.093 40.364 1.00 38.19
	ATOM	1575 CE1 HIS 412 44.357 4.150 39.363 1.00 34.75
45	ATOM	1576 NE2 HIS 412 43.659 5.263 39.474 1.00 35.52
	ATOM	1577 C HIS 412 46.264 4.932 44.793 1.00 46.35
	ATOM	1578 O HIS 412 46.326 5.951 45.479 1.00 42.73
	ATOM	1579 N HIS 413 47.049 3.883 44.993 1.00 48.92
	ATOM	1580 CA HIS 413 48.040 3.903 46.052 1.00 53.15
50	ATOM	1581 CB HIS 413 48.148 2.515 46.688 1.00 55.27

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ATOM 1582 CG HIS 413
                                46.843 2.015 47.238 1.00 58.77
     ATOM 1583 CD2 HIS 413
                                46.138 0.892 46.977 1.00 61.65
                                46.108 2.726 48.161 1.00 60.31
     ATOM 1584 ND1 HIS 413
                                45.003 2.061 48.445 1.00 63.01
     ATOM 1585 CE1 HIS 413
                                44.993 0.942 47.743 1.00 62.93
     ATOM 1586 NE2 HIS 413
                               49.359 4.364 45.456 1.00 53.19
     ATOM 1587 C HIS 413
     ATOM 1588 O HIS 413
                               50.335 3.617 45.390 1.00 54.93
     ATOM 1589 N VAL 414
                                49.343 5.612 44.999 1.00 53.77
     ATOM 1590 CA VAL 414
                                50.487 6.282 44.389 1.00 51.06
     ATOM 1591 CB VAL 414
                                50.374 6.305 42.838 1.00 51.49
10
     ATOM 1592 CG1 VAL 414
                                 51.603 6.958 42.231 1.00 45.22
     ATOM 1593 CG2 VAL 414
                                 50.210 4.891 42.304 1.00 52.67
     ATOM 1594 C VAL 414
                                50.444 7.724 44.894 1.00 54.28
     ATOM 1595 O VAL 414
                                49.418 8.401 44.774 1.00 55.49
15
     ATOM 1596 N THR 415
                                51.547 8.190 45.467 1.00 56.28
     ATOM 1597 CA THR 415
                                51.610 9.550 45.986 1.00 57.83
     ATOM 1598 CB THR 415
                                52.874 9.756 46.858 1.00 59.64
     ATOM 1599 OG1 THR 415
                                 52.922 11.115 47.311 1.00 66.69
     ATOM 1600 CG2 THR 415
                                 54.137 9.436 46.067 1.00 59.42
20
     ATOM 1601 C THR 415
                               51.599 10.577 44.855 1.00 56.98
     ATOM 1602 O THR 415
                               52.176 10.345 43.789 1.00 55.70
     ATOM 1603 N HIS 416
                               50.936 11.707 45.093 1.00 57.44
     ATOM 1604 CA HIS 416
                               50.835 12.786 44.108 1.00 57.34
     ATOM 1605 CB HIS 416
                               52.207 13.425 43.875 1.00 61.35
25
     ATOM 1606 CG HIS 416
                               52.860 13.940 45.123 1.00 69.78
     ATOM 1607 CD2 HIS 416
                                54.049 13.633 45.695 1.00 71.42
     ATOM 1608 ND1 HIS 416
                                52.283 14.901 45.922 1.00 72.49
     ATOM 1609 CE1 HIS 416
                                53.087 15.165 46.938 1.00 75.50
     ATOM 1610 NE2 HIS 416
                                54.165 14.410 46.819 1.00 73.91
     ATOM 1611 C HIS 416
30
                               50.301 12.260 42.773 1.00 53.79
     ATOM 1612 O HIS 416
                               50.769 12.667 41.710 1.00 52.81
     ATOM 1613 N PHE 417
                               49.318 11.366 42.824 1.00 48.05
     ATOM 1614 CA PHE 417
                                48.769 10.784 41.610 1.00 47.99
     ATOM 1615 CB PHE 417
                                47.652 9.799 41.940 1.00 46.11
35
     ATOM 1616 CG PHE 417
                                47.314 8.868 40.791 1.00 44.27
     ATOM 1617 CD1 PHE 417
                                48.155 7.796 40.481 1.00 41.79
     ATOM 1618 CD2 PHE 417
                                46.179 9.091 40.003 1.00 40.23
     ATOM 1619 CE1 PHE 417
                                47.872 6.936 39.386 1.00 44.30
                                45.874 8.248 38.907 1.00 36.80
     ATOM 1620 CE2 PHE 417
40
     ATOM 1621 CZ PHE 417
                                46.725 7.167 38.595 1.00 40.69
     ATOM 1622 C PHE 417
                               48.227 11.824 40.625 1.00 46.69
     ATOM 1623 O PHE 417
                               48.551 11.787 39.436 1.00 43.35
     ATOM 1624 N TRP 418
                               47,410 12,746 41,124 1,00 45,14
     ATOM 1625 CA TRP 418 · 46.821 13.775 40.276 1.00 44.89
45
     ATOM 1626 CB TRP 418
                                45.808 14.604 41.077 1.00 42.24
     ATOM 1627 CG TRP 418
                                45.096 15.646 40.259 1.00 47.11
     ATOM 1628 CD2 TRP 418
                                44.186 15.417 39.159 1.00 46.98
     ATOM 1629 CE2 TRP 418
                                43.786 16.678 38.676 1.00 48.94
     ATOM 1630 CE3 TRP 418
                                43.676 14.261 38.548 1.00 45.23
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     ATOM 1631 CD1 TRP 418
                                45.204 17.003 40.387 1.00 46.24
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	ATOM	1632 NE1 TRP 418	44.425 17.637 39.448 1.00 50.63
	ATOM	1633 CZ2 TRP 418	42.891 16.839 37.598 1.00 45.46
	ATOM	1634 CZ3 TRP 418	42.780 14.411 37.468 1.00 44.50
	ATOM	1635 CH2 TRP 418	42.403 15.696 37.009 1.00 47.55
5	ATOM	1636 C TRP 418	47.862 14.676 39.598 1.00 43.88
	ATOM	1637 O TRP 418	47.834 14.842 38.383 1.00 43.17
	ATOM	1638 N PRO 419	48.788 15.281 40.369 1.00 43.55
	ATOM	1639 CD PRO 419	49.006 15.290 41.826 1.00 41.52
	ATOM	1640 CA PRO 419	49.787 16.135 39.725 1.00 41.48
10	ATOM	1641 CB PRO 419	50.626 16.627 40.912 1.00 39.21
	ATOM	1642 CG PRO 419	49.593 16.667 42.017 1.00 39.25
	ATOM	1643 C PRO 419	50.616 15.363 38.701 1.00 36.28
	ATOM	1644 O PRO 419	50.940 15.882 37.638 1.00 37.08
	ATOM	1645 N LYS 420	50.959 14.124 39.033 1.00 35.96
15	ATOM	1646 CA LYS 420	51.742 13.281 38.132 1.00 40.82
	ATOM	1647 CB LYS 420	52.094 11.945 38.792 1.00 40.78
	ATOM	1648 CG LYS 420	53.086 12.046 39.933 1.00 48.62
	ATOM	1649 CD LYS 420	53.391 10.668 40.497 1.00 55.12
	ATOM	1650 CE LYS 420	54.395 10.741 41.635 1.00 53.26
20	ATOM	1651 NZ LYS 420	54.719 9.388 42.152 1.00 52.69
	ATOM	1652 C LYS 420	50.957 13.005 36.860 1.00 40.29
	ATOM	1653 O LYS 420	51.516 12.989 35.764 1.00 39.66
	ATOM	1654 N LEU 421	49.658 12.786 37.023 1.00 38.33
	ATOM	1655 CA LEU 421	48.784 12.507 35.903 1.00 37.60
25	ATOM	1656 CB LEU 421	47.417 12.074 36.428 1.00 43.66
	ATOM	1657 CG LEU 421	46.386 11.479 35.474 1.00 46.50
	ATOM	1658 CD1 LEU 421	46.946 10.253 34.770 1.00 45.15
-	ATOM	1659 CD2 LEU 421	45.154 11.107 36.279 1.00 51.31
	ATOM	1660 C LEU 421	48.661 13.747 35.014 1.00 39.59
30	ATOM	1661 O LEU 421	48.599 13.638 33.791 1.00 40.66
	ATOM	1662 N LEU 422	48.642 14.928 35.623 1.00 39.57
	ATOM	1663 CA LEU 422	48.545 16.170 34.867 1.00 38.63
	ATOM	1664 CB LEU 422	48.313 17.357 35.802 1.00 41.79
	ATOM	1665 CG LEU 422	46.996 17.407 36.581 1.00 42.74
35	ATOM	1666 CD1 LEU 422	47.010 18.606 37.515 1.00 42.89
	ATOM	1667 CD2 LEU 422	45.823 17.494 35.628 1.00 39.27
	ATOM	1668 C LEU 422	49.808 16.410 34.039 1.00 40.47
	ATOM	1669 O LEU 422	49.747 17.029 32.979 1.00 47.83
	ATOM	1670 N MET 423	50.949 15.936 34.519 1.00 34.27
40	ATOM	1671 CA MET 423	52.187 16.103 33.774 1.00 35.25
	ATOM	1672 CB MET 423	53.403 15.716 34.622 1.00 32.56
	ATOM	1673 CG MET 423	53.675 16.654 35.774 1.00 40.70
	ATOM	1674 SD MET 423	55.226 16.278 36.597 1.00 47.65
	ATOM	1675 CE MET 423	54.920 14.601 37.163 1.00 47.16
45	ATOM	1676 C MET 423	52.164 15.254 32.502 1.00 35.13
	ATOM	1677 O MET 423	52.934 15.499 31.570 1.00 29.85
	ATOM	1678 N LYS 424	51.285 14.252 32.482 1.00 31.56
	ATOM	1679 CA LYS 424	51.152 13.384 31.316 1.00 32.29
	ATOM	1680 CB LYS 424	50.373 12.115 31.681 1.00 30.56
50	ATOM	1681 CG LYS 424	51.106 11.178 32.631 1.00 30.07

	4 TO) (1692 CD LVC 424	52.248 10.482 31.938 1.00 33.22
	ATOM	1682 CD LYS 424	
	ATOM	1683 CE LYS 424	53.059 9.593 32.875 1.00 28.75 53.868 10.383 33.833 1.00 31.01
	ATOM	1684 NZ LYS 424	
_	ATOM	1685 C LYS 424	
5	ATOM	1686 O LYS 424	50.719 13.944 29.030 1.00 30.22
	ATOM	1687 N VAL 425	49.514 15.036 30.573 1.00 23.53 48.792 15.849 29.601 1.00 28.91
	ATOM	1688 CA VAL 425	=
	ATOM	1689 CB VAL 425	47.808 16.829 30.295 1.00 29.44
	ATOM	1690 CG1 VAL 425	47.148 17.737 29.273 1.00 28.81
10	ATOM	1691 CG2 VAL 425	46.744 16.049 31.057 1.00 31.22
	ATOM	1692 C VAL 425	49.822 16.669 28.831 1.00 32.03
	ATOM	1693 O VAL 425	49.771 16.769 27.605 1.00 31.95
	ATOM	1694 N THR 426	50.763 17.247 29.570 1.00 33.61
	ATOM	1695 CA THR 426	51.821 18.057 28.995 1.00 30.76
15	ATOM	1696 CB THR 426	52.678 18.695 30.105 1.00 32.34
	ATOM	1697 OG1 THR 426	51.842 19.535 30.912 1.00 33.07
	ATOM	1698 CG2 THR 426	53.812 19.533 29.514 1.00 25.40
	ATOM	1699 C THR 426	52.712 17.225 28.086 1.00 32.53
	ATOM	1700 O THR 426	53.113 17.686 27.014 1.00 35.19
20	ATOM	1701 N ASP 427	53.022 16.003 28.507 1.00 28.83
		1702 CA ASP 427	53.858 15.130 27.695 1.00 35.12
	ATOM	1703 CB ASP 427	54.273 13.880 28.476 1.00 39.14
	ATOM	1704 CG ASP 427	55.122 14.212 29.693 1.00 45.80
	ATOM	1705 OD1 ASP 427	56.052 15.034 29.556 1.00 41.97
25	ATOM	1706 OD2 ASP 427	54.869 13.642 30.775 1.00 50.06
	ATOM	1707 C ASP 427	53.124 14.726 26.422 1.00 33.94
	ATOM	1708 O ASP 427	53.737 14.617 25.362 1.00 38.02 51.818 14.512 26.529 1.00 27.15
	ATOM	1709 N LEU 428	51.013 14.148 25.373 1.00 29.99
• •	ATOM	1710 CA LEU 428	
30	ATOM	1711 CB LEU 428	49.602 13.719 25.802 1.00 22.49 49.541 12.285 26.359 1.00 25.54
	ATOM	1712 CG LEU 428	49.541 12.285 26.359 1.00 25.54 48.210 12.021 27.037 1.00 20.60
	ATOM	1713 CD1 LEU 428	49.785 11.303 25.224 1.00 17.24
	ATOM	1714 CD2 LEU 428	
	ATOM	1715 C LEU 428	
35	ATOM	1716 O LEU 428	50.941 15.088 23.174 1.00 31.26 50.910 16.531 24.887 1.00 27.64
	ATOM	1717 N ARG 429	50.877 17.694 24.011 1.00 28.13
	ATOM	1718 CA ARG 429	50.584 18.969 24.800 1.00 29.59
	ATOM	1719 CB ARG 429	49.224 18.980 25.455 1.00 34.85
40	ATOM	1720 CG ARG 429	48.951 20.314 26.118 1.00 47.18
40	ATOM	1721 CD ARG 429	47.657 20.358 26.797 1.00 57.93
	ATOM		46.473 20.193 26.200 1.00 63.62
	ATOM	1723 CZ ARG 429	
	ATOM	1724 NH1 ARG 429 1725 NH2 ARG 429	
15	ATOM		52.229 17.819 23.304 1.00 22.81
45	ATOM	1726 C ARG 429 1727 O ARG 429	52.294 18.209 22.143 1.00 30.81
	ATOM	1727 O ARG 429 1728 N MET 430	53.305 17.482 24.008 1.00 30.81
	ATOM	1728 N MET 430 1729 CA MET 430	54.639 17.545 23.422 1.00 34.72
	ATOM ATOM		55.716 17.323 24.485 1.00 34.97
50	ATOM		55.864 18.480 25.451 1.00 45.34
50	AIOM	1/31 CG ME1 430	JJ.007 10.700 ZJ.7J1 1.00 7J.J7

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	ATOM	1732 SD MET 430	56.162 20.050 24.596 1.00 52.55
	ATOM	1733 CE MET 430	57.598 19.639 23.589 1.00 55.56
	ATOM	1734 C MET 430	54.778 16.500 22.325 1.00 34.01
	ATOM	1735 O MET 430	55.440 16.733 21.318 1.00 37.29
5	ATOM	1736 N ILE 431	54.161 15.340 22.533 1.00 29.99
	ATOM	1737 CA ILE 431	54.197 14.279 21.545 1.00 28.82
	ATOM	1738 CB ILE 431	53.523 12.984 22.095 1.00 27.39
	ATOM	1739 CG2 ILE 431	53.260 11.989 20.956 1.00 23.87
	ATOM	1740 CG1 ILE 431	54.414 12.386 23.201 1.00 25.56
10	ATOM	1741 CD1 ILE 431	53.850 11.155 23.896 1.00 17.29
	ATOM	1742 C ILE 431	53.450 14.785 20.301 1.00 29.49
	ATOM	1743 O ILE 431	53.908 14.603 19.174 1.00 24.19
	ATOM	1744 N GLY 432	52.311 15.435 20.524 1.00 25.25
	ATOM	1745 CA GLY 432	51.542 15.971 19.419 1.00 30.38
15	ATOM	1746 C GLY 432	52.334 16.997 18.614 1.00 32.75
	ATOM	1747 O GLY 432	52.410 16.895 17.387 1.00 36.38
	ATOM	1748 N ALA 433	52.930 17.974 19.294 1.00 26.77
	ATOM	1749 CA ALA 433	53.711 19.012 18.625 1.00 26.48
	ATOM	1750 CB ALA 433	54.182 20.047 19.631 1.00 19.90
20	ATOM	1751 C ALA 433	
	ATOM	1752 O ALA 433	55.207 18.787 16.760 1.00 31.60
	ATOM	1753 N CYS 434	55.582 17.467 18.537 1.00 33.22
	ATOM	1754 CA CYS 434	56.728 16.801 17.914 1.00 34.34
	ATOM	1755 CB CYS 434	57.339 15.808 18.895 1.00 35.20
25	ATOM	1756 SG CYS 434	59.191 15.745 18.798 1.00 54.48
	ATOM	1757 C CYS 434	56.313 16.052 16.636 1.00 34.09
	ATOM	1758 O CYS 434	57.095 15.937 15.679 1.00 34.89
	ATOM	1759 N HIS 435	55.088 15.545 16.642 1.00 34.30
	ATOM	1760 CA HIS 435	54.570 14.818 15.501 1.00 35.44
30	ATOM	1761 CB HIS 435	53.296 14.061 15.886 1.00 31.76
	ATOM	1762 CG HIS 435	52.587 13.469 14.715 1.00 32.03
	ATOM	1763 CD2 HIS 435	52.735 12.277 14.092 1.00 28.61
	ATOM	1764 ND1 HIS 435	51.665 14.177 13.970 1.00 28.48
	ATOM	1765 CE1 HIS 435	51.284 13.453 12.941 1.00 33.27
35	ATOM	1766 NE2 HIS 435	51.920 12.284 12.985 1.00 31.57
	ATOM	1767 C HIS 435	54.311 15.750 14.319 1.00 32.74
	ATOM	1768 O HIS 435	54.504 15.363 13.175 1.00 32.87
	ATOM	1769 N ALA 436	
	ATOM	1770 CA ALA 436	53.628 17.966 13.571 1.00 29.91
40	ATOM		53.221 19.290 14.197 1.00 21.23
	ATOM	1772 C ALA 436	54.911 18.135 12.769 1.00 33.86
	ATOM	1773 O ALA 436	54.892 18.128 11.541 1.00 36.10
	ATOM	1774 N SER 437	56.030 18.266 13.483 1.00 35.19
	ATOM	1775 CA SER 437	57.344 18.426 12.871 1.00 33.03
45	ATOM	1776 CB SER 437	58.389 18.720 13.941 1.00 35.31
	ATOM	1777 OG SER 437	59.681 18.782 13.373 1.00 44.99
	ATOM	1778 C SER 437	57.758 17.178 12.100 1.00 38.39
	ATOM	1779 O SER 437	58.374 17.269 11.034 1.00 37.54
	ATOM	1780 N ARG 438	57.427 16.012 12.642 1.00 37.32
50	ATOM	1781 CA ARG 438	57.762 14.754 11.992 1.00 39.30

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57.517 13.572 12.941 1.00 42.97
    ATOM 1782 CB ARG 438
                                58.542 13.436 14.059 1.00 41.72
    ATOM 1783 CG ARG 438
                                59.926 13.212 13.484 1.00 45.23
    ATOM 1784 CD ARG 438
                                59.961 12.050 12.601 1.00 45.66
    ATOM 1785 NE ARG 438
                                60.935 11.804 11.731 1.00 49.71
    ATOM 1786 CZ ARG 438
                                61.961 12.641 11.627 1.00 50.91
    ATOM 1787 NH1 ARG 438
                                60.885 10.727 10.960 1.00 46.86
    ATOM 1788 NH2 ARG 438
                               56.939 14.565 10.725 1.00 42.37
    ATOM 1789 C ARG 438
                               57.311 13.794 9.841 1.00 40.58
    ATOM 1790 O ARG 438
    ATOM 1791 N PHE 439
                               55.816 15.269 10.645 1.00 42.25
10
                               54.957 15.170 9.479 1.00 42.81
    ATOM 1792 CA PHE 439
                               53.593 15.790 9.771 1.00 42.18
    ATOM 1793 CB PHE 439
                               52.594 15.597 8.656 1.00 42.48
    ATOM 1794 CG PHE 439
                                52.173 14.312 8.295 1.00 47.09
    ATOM 1795 CD1 PHE 439
                                52.086 16.696 7.961 1.00 39.76
    ATOM 1796 CD2 PHE 439
15
                                51.256 14.110 7.234 1.00 49.17
    ATOM 1797 CE1 PHE 439
                                51.174 16.524 6.896 1.00 45.10
    ATOM 1798 CE2 PHE 439
                               50.751 15.225 6.532 1.00 46.36
    ATOM 1799 CZ PHE 439
    ATOM 1800 C PHE 439
                               55.626 15.905 8.322 1.00 44.79
                               55.596 15.444 7.181 1.00 40.26
    ATOM 1801 O PHE 439
20
    ATOM 1802 N LEU 440
                               56.236 17.049 8.629 1.00 42.77
                                56.927 17.839 7.621 1.00 42.96
    ATOM 1803 CA LEU 440
                                57.421 19.156 8.216 1.00 37.19
    ATOM 1804 CB LEU 440
                                56.348 20.117 8.725 1.00 36.97
    ATOM 1805 CG LEU 440
                                57.020 21.338 9.321 1.00 33.65
     ATOM 1806 CD1 LEU 440
25
                                55.411 20.519 7.572 1.00 35.42
    ATOM 1807 CD2 LEU 440
                               58.106 17.063 7.053 1.00 45.47
    ATOM 1808 C LEU 440
     ATOM 1809 O LEU 440
                               58.421 17.191 5.876 1.00 52.48
     ATOM 1810 N HIS 441
                              58,760 16.266 7.890 1.00 49.15
                               59.893 15.473 7.435 1.00 54.76
    ATOM 1811 CA HIS 441
30
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                               61.515 16.026 9.323 1.00 62.73
     ATOM 1813 CG HIS 441
                                62.851 16.166 9.508 1.00 65.73
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                               60.929 17.098 9.966 1.00 66.01
     ATOM 1815 ND1 HIS 441
                               61.871 17.845 10.518 1.00 65.55
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     ATOM 1817 NE2 HIS 441
                              59.417 14.292 6.589 1.00 55.93
     ATOM 1818 C HIS 441
                              60.084 13.908 5.630 1.00 57.33
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                               58.271 13.716 6.948 1.00 57.81
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                                57.712 12.585 6.203 1.00 59.11
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                                56.562 11.924 6.978 1.00 55.93
                                56.961 11.246 8.276 1.00 58.52
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     ATOM 1824 SD MET 442
                                54.430 11.779 9.350 1.00 52.61
     ATOM 1825 CE MET 442
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                                56.038 14.871 3.669 1.00 64.90
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     ATOM 1831 CG LYS 443
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                               52.879 12.197 -1.403 1.00 78.24
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                               52.647 13.459 -2.261 1.00 81.33
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    ATOM 1865 OG1 THR 448
                               52.552 13.087 -3.643 1.00 84.46
                                53.802 14.444 -2.089 1.00 83.51
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                                50.720 9.375 -2.783 1.00 75.03
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                               50.445 8.421 -1.622 1.00 73.49
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     ATOM 1875 CA LEU 450
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    ATOM 1878 CD1 LEU 450
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    ATOM 1951 CD2 PHE 459
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                                46.536 21.511 7.724 1.00 78.99
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                                47.014 23.786 7.237 1.00 87.62
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     ATOM 1978 C12 TRI
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     ATOM 1979 C13 TRI
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	ATOM	1984 O3 TRI 1	44.546 5.255 17.329 1.00 54.78	
_	ATOM	1985 O2 TRI 1	50.831 5.617 14.667 1.00 28.44	
5	ATOM	1986 O1 TRI 1	52.207 10.160 11.342 1.00 43.65	
	ATOM	1987 O4 TRI 1	44.021 3.333 18.352 1.00 42.95	4.0
	ATOM	1 AS CAC 501	60.548 16.977 16.916 1.00 65.97	AS
	ATOM	2 AS CAC 502	27.863 16.627 16.796 1.00 89.34	AS
	ATOM	3 AS CAC 503	29.889 28.698 21.811 1.00100.00	AS
10	ATOM	4 AS CAC 504	33.547 24.203 8.880 1.00100.00	AS
	ATOM	5 O HOH 505	42.365 8.872 4.597 1.00 53.88	HOH
	ATOM	6 O HOH 506	33.545 30.973 24.585 1.00 40.33	НОН
	ATOM	7 O HOH 507	37.040 1.824 12.671 1.00 61.87	HOH
	ATOM	8 O HOH 508	44.105 4.635 6.023 1.00 40.68	HOH
15	ATOM	9 O HOH 509	52.686 13.817 -6.263 1.00 54.00	HOH
	ATOM	10 O HOH 510	50.186 12.691 -5.997 1.00 55.36	НОН
	ATOM	11 O HOH 511	49.278 18.540 14.006 1.00 34.79	НОН
	ATOM	12 O HOH 512	25.541 28.885 21.206 1.00 55.42	НОН
	ATOM	13 O HOH 513	27.346 31.063 27.398 1.00 58.30	HOH
20	ATOM	14 O HOH 514	40.790 19.192 39.234 1.00 50.35	НОН
	ATOM	15 O HOH 515	37.467 0.637 37.293 1.00 37.46	HOH
	ATOM	16 O HOH 516	36.155 3.879 47.189 1.00 61.37	НОН
	ATOM	17 O HOH 517	35.410 5.865 50.995 1.00 63.46	НОН
	ATOM	18 O HOH 518	33.622 5.440 47.570 1.00 53.87	HOH
25	ATOM	19 O HOH 519	64.787 6.888 11.882 1.00 51.15	НОН
	ATOM	20 O HOH 520	61.109 -8.688 27.722 1.00 61.70	HOH
	ATOM	21 O HOH 521	49.869 -5.472 30.343 1.00 40.50	HOH
	ATOM	22 O HOH 522	43.786 -0.987 26.878 1.00 52.16	HOH
••	ATOM	23 O HOH 523	41.604 2.361 26.985 1.00 47.90	НОН НОН
30	ATOM	24 O HOH 524	54.405 6.361 39.795 1.00 56.56	НОН
	ATOM	25 O HOH 525	46.088 0.770 33.095 1.00 74.24	HOH
	ATOM	26 O HOH 526	50.481 16.245 15.314 1.00 28.99 59.788 14.863 21.416 1.00 50.02	НОН
	ATOM	27 O HOH 527		НОН
2.5	ATOM	28 O HOH 528	49.282 19.490 32.191 1.00 41.61 56.683 10.961 26.733 1.00 34.20	НОН
35	ATOM	29 O HOH 529		НОН
	ATOM	30 O HOH 530		НОН
	ATOM	31 O HOH 531	26.487 13.273 30.591 1.00 43.94 27.019 25.052 28.330 1.00 54.97	НОН
	ATOM	32 O HOH 532		НОН
40	ATOM	33 O HOH 533	50.689 1.918 29.551 1.00 30.63	
40	ATOM	34 O HOH 534	47.867 0.200 31.330 1.00 43.14	НОН НОН
	ATOM	35 O HOH 535	61.434 -0.721 23.218 1.00 49.83	НОН
	ATOM	36 O HOH 536	41.969 20.017 20.894 1.00 27.00 46.897 16.244 15.992 1.00 31.50	НОН
	ATOM	37 O HOH 537	29,796 16.276 27.000 1.00 38.52	НОН
4.5	ATOM	38 O HOH 538		НОН
45	ATOM	39 O HOH 539	47.853 23.205 20.217 1.00 44.39	
	ATOM	40 O HOH 540	40.956 24.775 31.717 1.00 50.36	HOH HOH
	ATOM	41 O HOH 541	43.310 1.560 41.912 1.00 43.56	поп
	END			

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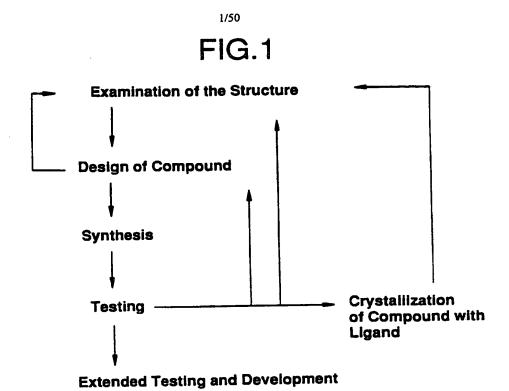


FIG.2

DOMAINS : NH2-TERMINAL	DNA BINDING	LIGAND BINDING
HOMOLOGY: Hypervariable	> 40%	About 20%
FUNCTION: Transactivation	DNA Binding Dimerization	LIGAND Binding Dimerization Transactivation Nuclear translocatio Hsp binding

	wo	99	/26	96	6
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	•	•	•	•	•	•	•	•	•	•	•		TSUTTENSA		DENNIMETAN	•		
	•	•	•	•	•	•	•		•	•	•	•		בשיים בי בי בי בי	RSSLGPTERT	•	<	4
	•	•	•	•	• • • • • • • • • • • • • • • • • • • •	• • • • • • • • • • • • • • • • • • • •	•	•	•	•	•	•		FEVGSFLLCR	SLPEGLDMER RWGQVSQAVE		[FIG. 3A
	•	•	•	•	•	•	•	•			•	•		MIELKAKGPR APHVAGGPPS		•		
-	•	• • • • • • • • • • • • • • • • • • • •	•	•	•	•	•	•	•	•	•	•		HTELKAKGPR	HETKGYH	•		
	rTRalpha	hTRalpha	hTRbeta	hRARalpha	hRARgamma	hRXRalpha	hRXRbeta	hPPARalpha	hPPARbeta	hPPARgamma	hvdr	her	hGR	hPR	hMR	hAR		

SUBSTITUTE SHEET (RULE 26)

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3/50 120 LDSVLDTLLA SATVAESHGL YHDSVRDADY VMDFYKTLÅG SSVLAQERGD SSPPEKDSGL SLTPGREENP EATRGAGGSS NNRPGILTSD IKTELESKEL SDVEGAYSRA MDSKE QELLPCLQQD DEKTODOQSL PRPCQGQDPS NSTOCSSKEK 61 hvdr hER hGR hPR PAR. hPPARgamma 1PPARalpha hPPARbeta hTRalpha hRXRalpha hRXRbeta hTRbeta hRARalpha hRARgamma

							,	4/50)							
180	•	•	•	•	•	•	•	•	•	•	•	•	.DSKQRRLLV DFPKGSVSNA	KVGDSSGTAA	SDSGSSVNGG	•
	•	•	•	•	•	•	•		•	•	•	•	.DSKQRRLLV	PPAAPATORV LSPLMSRSGC KVGDSSGTAA	NTPLRSFM	
	•	•	•	•	•		•	•	•	•	•	• • • • • • • • • • • • • • • • • • • •	•	PPAAPATORV	GHRPSTLSCV	•
	•	•	•	•	•	• • • • • • • • • • • • • • • • • • • •	•	•	• • • • • • • • • • • • • • • • • • • •	• • • • • • • • • • • • • • • • • • • •	• • • • • • • • • • • • • • • • • • • •	•	•	PSGPGQSQPS PPACEVTSSW CLFGPELPED	SYEQQNQQGS HSPAKIYQNV EQLVKFYKGN	•
	•	•	•	•	•	•	•	•	•	•	•	•	PSLAVASQS.	PPACEVTSSW	HSPAKIYONV	•
121	•	•	•	•	•	•	•	•	•	•	•	•	GATUKUSASS PSLAVASQS.	PSGPGQSQPS	SYEQQNQQGS	•
	rTRalpha	hTRalpha	hTRbeta	hRARa 1 pha	hRARgamma	hRXRa1pha	hRXRbeta	hPPARalpha	hPPARbeta	hPPARgamma	hVDR	her	hgR	hPR	hMR.	hAR

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SSTIASFGSF PVHSPITQGT ESAGPLLKGK ESIANLNRS. SGETDLKLLE VEEEDSSESE ESPHWSGAPV KPSPQAAAVE FPQQCQISLS VHRAIVK .. S PIHCHEKSPS VCSPLNHTSS VCSPAGINSV ETKVMGNDLG PARQLLLPAS QQPDLSKAVS LSHGLYHGET AHKVLPRGLS 181 hvdr her hGR hPR HA HA rTRalpha hTRalpha hTRbeta hPPARgamma hRASalpha hRARgamma hRXRalpha hRXRbeta hPPARalpha hPPARbeta

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6/50 300 PVSSPNNVIL GNVKLYTT. HLKGQTGTNG EDSRESAPRV ALVEQDAPMA SPPSHCSVKS THSDVSSEQQ RGSRSHSPAH ASNVGSPLSS PLSSHKSSIS PKSSASTAVS AAPTEKEFPK GGAAACPPGA AAGGVALVPK PLICSPNAEN ...TSVPEN PRALCGAAAG 241 hGR hPR hvdr her HAR HAR hPPARalpha hPPARbeta hPPARgamma hRXRalpha hRXRbeta hTRalpha hRARgamma rTRalpha hTRbeta hRARa I pha

						7	/50										
360	•	•	•	•	•	•	•	• • • • • • • • • • • • • • • • • • • •	•	•	•		NESPWRSDLL	SA FAPPRTSPCA	TASGTSAGSS	•	
	•	•	•	•		•	•	•	•		•	• • • • • • • • • • • • • • • • • • • •	ET	SA	CSPVNNAFSY TASGISAGSS	•	
	•	•	•	•	•	•	•	•	•	•	•	•	SGSPGK	GGAGAA	SPAASTVGSI	•	٦c
	•	•	•			•	•	•	•	•	•	•	DQST FDILQDLEFS	ROLLEDESYD	NNSRCSVSSP SNTNNRSTLS	•	
		•	•	•	•	•	•	•	•	•	•	•	bosr	LNHALLAART	NNSRCSVSSP	•	
301	•	•	•	•	•	•	•	•	•		•	•	•	HDFIHVPILP LNHALLAART	RSSVSSPANI	•	
	rTRalpha	hTRalpha	hTRbeta	hRARalpha	hRARgamma	hRXRalpha	hRXRbeta	hPPARalpha	hPPARbeta	hPPARgamma	hvdr	her	hGR	hPR	har	har	

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8/50 ILPDIKPKIK DNGDLVLSSP SNVTLPQVKT SARSPRSYLV TQEKGAQEVP FPKTEEVESA ISNGVIGQLN IVQYIKPEPD GAFSSSCLGG 420 MSW AARPPFLPQR HAEGSVGRWG YSDFQPPALK IKEEEEGAEA AEPKDDAYPL GNSNEDCKPL AGEDDSFLLE P. DCAYPPD SSTPVAVGDF TLRDWVPSPD IDENCLLSPL 361 hGR her hPR hVDR FAR. hRARgamma **hRXRalpha** hRXRbeta hPPARalpha hPPARbeta hPPARgamma rTRalpha hTRalpha hTRbeta hRARalpha

FIG.3H

9/50 480 **MSAISVHGVS PASASVSSAS** KDYYSLSGIL TIRVLEVEVD YPEGAAYEFN SRSPDSSSPNGA VAPYGYTRP. FSTQVNSS.AA SVPIKQESTK HSCSGTSFKG NPTVNPFPFH DGSYFSFMDD AQVIVMSGQE PLERPLGEVY LDSSKPAVYN XN.... **HDTKHFLPLD** RDGRH..CRD SCILKFPAQD GGGGRRRIIN PGAGARGWIGGG GGGEA.... EAAVT ANIIG.... TVYCQASFPG PLTVNEQLLG EPLNRPQLKI PR.ATPSRPG DTEDLPANNA PGVIKQEKLG AKECIVGSAT ALAGSRSGGG LLHQIQGNEL FPLGPPPPLP **X** TLHTKASGMA AGANPAAFPD NSKINSDSSF EKEDFIELCT 421 hGR her hPR **HHR** hPPARgamma hvdr **hAR** hRXRbeta hPPARbeta hRARgamma hRXRalpha hPPARalpha rTRalpha hTRa1pha hTRbeta hRARa 1 pha

10/50

	481					540
rTRalpha	•		•	•	HEQKPSK	VECGSDPEEN
hTRalpha	•		•	•	HEQKPSK VECGSDPEEN	VECGSDPEEN
hTRbeta	•		MTPNSHTE	NGLTAWDKPK	HCPDREHDWK	LVGHSEACLH
hRARalpha	• • • • • • • • • • • • • • • • • • • •		•	•	• • • • • • • • • • • • • • • • • • • •	•
hRARgamma	•		•	X	ATNKERLFAA	GALGPGSGYP
hRXRalpha	.LISPIGR	LISPICR GSMAAPSLHP SLGPGIGSPG .QLHSPISTL SSPINGMGPP FSVISSPHGP	SLGPGIGSPG	.QLHSPISTL	SSPINGHGPP	FSVISSPHGP
hRXRbeta	PLPOGVPP	PLPOGVPP PSPPGPPLPP STAPTLGGSG .APPPP PMPPPPLGSP FPVISSSMGS	STAPTLGGSG	APPPP	PMPPPPLGSP	FPVISSSHGS
hPPARalpha	HVDTESPL	MVDTESPL CPLSPLEAGD LESPLSEEFL QEMGNIQEIS QSIGEDSSGS FGFTEYQYLG	LESPLSEEFL	QEMGNIQEIS	QSIGEDSSGS	FGFTEYQYLG
hPPARbeta	•	HEQPQ EEAP EVREEEEKE EVAEAEGAPE LNGGPQHALP	EEAP	. EVREEEEKE	EVAEAEGAPE	LNGGPQHALP
hPPARgamma	•		TEMPFWPTNF	GISSVD	LSMADDHSHS	FDIKPFITVD
hVDR	TALSSAGAAE	TALSSAGAAE SGGDEEGSGQ SLEATEEAQL DGPVTTSSTT AVTVEVSAPV VQTVVSKAAI	SLEATEEAQL	DGPVTTSSTT	AUTVEVSAPV	VQTVVSKAAI
her	AAAAANAOVY	AAAAANAQVY GQTGLPYGPG SEAAAFGSNG LGGFPPLNSV SPSPLMLHP PPQLSPFLQP	SEAAAFGSNG	LGGFPPLNSV	SPSPLMLHP	PPQLSPFLQP
hgR	TSGGQHYHYD	TSGGOMYHYD HNTASLSQQQ DQ KPIFNVIPP IPVGSEN	DQ	.KPIFNVIPP	IPVGSEN	•
hPR	SSGSTLECIL	SSGSTLECIL YKAEGAPPQQ GPFAPPCKA PGASGCLLPR DGLPSTS	GPFAPPPCKA	PGASGCLLPR	DGLPSTS	•
har.	GPPVPGFDGN	GPPVPGFDGN CEGSGFPVGI KQEPDDGSYY PEASIPSSAI VGVNSGGQSF HYRIGAQGTI	KQEPDDGSYY	PEASIPSSAI	VGVNSGGQSF	HYRIGAQGTI
hAR	•	PQGLAGQE SDFTAPDVWY PGGHVSR VPYPSPT	SDFTAPDVWY	PGGHVSR	VPYPSPT	•

FIG.3

							11	/50										
009	SGYI	SGX I	TEEKKCKGYI	EEIVPSPPSP	EEHVPSSPSP	VLKVPAHPSG	GLHCPPPPGG	YPWVPGSVDE	sepp str notonge. De	A OF WARDHER		Section 1	DNGSTATION	SSFFSSSSI	DSEASQSPQY	NTIVESHKSH GDLSSRRSDG YPVLEYIPEN VSSSTLRSVS		
	•	SGX I	QSVSSAQTFQ	AAIETQSSSS	LSVETQSTSS	DIKPPLGLNG	DVKPPVLGVR	SSPS. SVT	cepp str	######################################	PASPELLSEN	GOPLLIPLSM	GGRERLASIN	V	YPPYLNYLRP	YPVLEYIPEN	TO TOVED	
	•	•	FHLDHDDVND	SNHVASGAGE	OPDLPKEMAS	PHNPVSSSE	TPCCCSCPPE	SAFALLING LESS TO SEPTEMBER APPROPRIES	•		QEYQSAIKVE	TCHLAQQSSL	YRPNSDNRRQ	CYSSPSHRPD	AVLKEGLPQV	GDLSSRRSDG		MKLETARUHV
	LKSSM	LKTSH	LIQTIWISSI	Nd	MISPSFRGLG	CSPOTSS	STANTOGSS	SSECTIONS	•	•	VADYKYDLKL	LTQDGLASLH	AGPPAF	NFPGRTVFSN	NGLPQLGYQA	NTLVESWKSH		DYGD
	RKN.GQCP	RKN.GQCS	LKN. EOSSPH	PN SNHVASGAGE AAIETQSSSS EEIVPSPPSP	GROOD OTE	AMPLES DIRPLEING VLKVPAHPSG	TITITUTES CENTREMY I DECESCIONE DURPPULGUR GLHCPPPGG	. APPGFSGFV	TDTLSPA	LSRS	DIPFTRADPH	PITVQACPQV	NEPSGYTVRE	WARCOCSC DONLISLGIL NFPGRIVESN GYSSPSMRPD V SSPESSES	ASABABGA APALYPALGI NGLPQLGYQA AVIKEGLPQV YPPYLNYLRP DSEASQSPQY	FOUT CCFDDV	SLSKSAKOVS FYRESSILLI	. CVKSEMGP WMDSYSGPYGD MKLEIAKDHV LF.: LDIII: :::
541	SARSPOGKRK RKN.GQCP	SARSPOGKRK RKN.GQCS	PRCHERRST LKN. EOSSPH LIQITMISSI FHLDHDDVND QSVSSAQIFQ TEEKKCKGII		CONTRACTOR AT D. CODDER WISPSFRGLG OPDIPKEMAS LSVETQSTSS EEHVPSSPSP	CAGEFFAFF	HSMSVF		SCPGSDGSVI	SSSYTDLSRS	FSSISAPHYE DIPFTRADPM VADYKYDLKL QEYQSAIKVE PASFIISEN AKLININING	SVSPAQQTSV PITVQACPQV LTQDGLASLH TGHLAQQSSL GQPLLIPLSH AGSVGGGGG	HCOOVPYYLE NEPSGYTVRE AGPPAF YRPNSDNRRQ GGREKLASIN DAGSGARESS	CANACOGSC	ACKARASA.		SLSKSAKUŲS	CVKSEMGP
	rTRalpha	hTRalpha	A TOPOTA	nirwera.	hRARa I pna	hRARgamma	hRXRalpha	hRXRbeta	hPPARalpha	hPPARbeta	hPPARgamma	hvdR	her	ָ בּ בּ	אסמא	וובע	A.A.	hAR

12/50 099 QAVLQPQMSA DL..... DK TN.... DR. DL..TYSCRD NK. NH..VYTCHR KLIYD...RC HN. DYMCPA KLVYD...KC KLEYE...KC QHNYLCAGRN NLHPTYSCKY NLHPTYSCKY NLHPSYSCKY NH.. VYTCHR DL..TYTCRD SVOTOLOAPA **QHNYLCAGRN** QHNYLCAGRN KOKYLCASRN KGFFRRSIQK KGFFRRTIOK HYRCITCEGC KGFFRRTIQK KGFFRRTIQK KAFFKRSIQG HYGALTCGSC KVFFKRAAEG KGFFRRSIQK KGFFKRTVRK KGFFRRTIRL KGFFRRTIRM KGFFRRTIRL AGLQAATVLN KVFFKRAVEG KVFFKRAMEG KVFFKRAVEG KGFFKRTIRK HY RCITCEGC HYGVSSCEGC HYGVWSCEGC HYGVLTCGSC HYGWYCGSC HYRCITCEGC HYGVSACEGC HYGVYSCEGC HYGVYSCEGC HYGVHACEGC HYGVHACEGC HYGVLTCGSC HYGVHACEGC PAGGLLKLPF WCGDKATGY **FVCNDKSSGY** AICCDRSSGK LICCDEASGC LVCGDEASGC LICGDKASGC WCGDKATGY RICCDKASGY LVCSDEASGC FVCQDKSSGY AICGDRSSGK RVCGDKASGF RVCGDKASGF ATLPGLAAAS AVCNDYASGY WCGDKATGY ATTGPPPKLC SFESLPOKIC NHASFTKHIC SPSGALNIEC IGSSRPSKICPQKTC PSYLDKDELC PPLPRIYKPC PPPPRVYKPC PGAG..KRLC AVLTLPTATV KET...RYC PSYLDKDEQC PSYLDKDEQC ASCGSLNMEC PSNSLMAIEC 601 hvdr her hGR hPR hRXRalpha hPPARgamma HAR A rTRalpha hTRalpha hTRbeta hRARalpha hRARgamma hRXRbeta hPPARalpha hPPARbeta

FIG.3K

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VLDDSKRVAK VLDDSKRLAK VLDDSKRLAK VRND VQEERQRG VQEERQRG IRFG IRFG IRFG IRFG IRFG	RKSKKLGKLN GIHEEQFQ	
NKITR NGCQLCRFKK CIAVGMAMDL VLDDSKRVAK RKLIEQNRER NKUTR NQCQLCRFKK CIAVGMAMDL VLDDSKRLAK RKLIEGNRER NKVTR NQCQECRFKK CIYVGMATDL VLDDSKRLAK RKLIEENREK IKVTR NRCQYCRLQK CFEVGMSKES VRNDRNK NKVTR NRCQYCRLQK CFEVGMSKEA VRNDRNK NKOQYCRYQK CLAMGMKREA VQEERQRGKDK.DG NKRQR NRCQYCRYQK CLATGMKREA VQEERQRGRDR.DG NKRNR NKCQYCRFQK CLATGMKREA VQEERQRGRMPRAEKRK NKCQYCRFQK CLAUGMSHNA IRFGRMPRAEKRK NKCQYCRFQK CLAUGMSHNA IRFGRMPQAEKEK NKCQYCRFQK CLAUGMSHNA IRFGRMPQAEKEK NKCQYCRFQK CLAUGMSHNA IRFGRMPQAEKEK NKCQYCRFQK CLAUGMSHNA IRFGRMPQAEKEK NKCYCRFQK CLAUGMSHNA IRFGRMFRRQRDGG NKIRR KSCQACRLRK CYEVGMHKGG IRKDRRGGRM LKHKRQRDDG NKIRR KNCPACRLRK CYEVGMHKGGRKFKKFNNKVR	KKLGNLK	
KITR NQCQLCRFKK CIAVGMAMDL VLDDSKRVAK)KITR NQCQLCRFKK CIAVGMAMDL VLDDSKRVAK)KVTR NQCQECRFKK CIYVGMATDL VLDDSKRLAK IKVTR NRCQYCRLQK CFEVGMSKES VRND IKVTR NRCQYCRLQK CFEVGMSKEA VRND IKVTR NRCQYCRYQK CLAMGMKREA VQEERQRG IKRQR NRCQYCRYQK CLATGMKREA VQEERQRG IKKSR NKCQYCRFQK CLATGMSHNA IRFG IKKSR NKCQYCRFQK CLAVGMSHNA IRFG ITQTT AATTASIVQK ASEPSVSVAT LQTAGLSINP IKNRR KSCQACRLRK CYEVGMMKGG IRKDRRGGRM IKIRR KNCPACRYRK CLQAGMNLEA IKIRR KNCPACRIRK CCQAGMVLGG	3 3	
NITR NGCQLCRFKK CIAVGMAMDL NKITR NQCQLCRFKK CIAVGMAMDL NKVTR NQCQECRFKK CIYVGMATDL IKVTR NRCQYCRLQK CFEVGMSKES IKVTR NRCQYCRLQK CFEVGMSKEA NKRQR NRCQYCRYQK CLAMGMKREA NKRQR NRCQYCRYQK CLAMGMKREA NKRQR NRCQYCRFQK CLALGMSHNA NKYRR NKCQYCRFQK CLAUGMSHNA NKYRR NKCQYCRFQK CLAUGMSHNA NKYRR KSCQACRLRK CYEVGHMKGG NKIRR KNCPACRYRK CYEVGHMKGG NKIRR KNCPACRYRK CLQAGHNLEA NKIRR KNCPACRIRK CCQAGHVLGG		
KITR NGCQLCRFKK KITR NQCQLCRFKK KVTR NQCQECRFKK KVTR NRCQYCRLQK KVTR NRCQYCRLQK KRQR NRCQYCRYQK KKNR NRCQYCRYQK KKNR NKCQYCRFQK KKNR KSCQACRLRK KRIGR KNCPACRLRK	CLQAGMNLGA CYEAGMTLGA	
KITR OKITR IKVTR IKVTR IKVTR IKVTR IKKOR OKROR IKKSR IKKSR IKKSR IKKSR IKKSR IKKSR IKKSR IKKSR IKKSR	CIIDKIRR KNCPACRLOK CLOAGHNLGA CTIDKFRR KNCPSCRLRK CYEAGHTLGA	
661 CCCVID CCCVID NCIIN NCIIN DCLID DCLID SCKIQ SCKIQ NCRIH LQAMQC CCTIC CIVI	CIIDKIRR CTIDKFRR	
rTRalpha hTRalpha hTRbeta hRARgamma hRARgamma hRXRalpha hPPARalpha hPPARalpha hPPARalpha hPPARalpha hPPARGamma hPPARGamma	har har	

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14/50 780 IHDIETLWOA IYDHNSLHHG INDMETICHA LL.... LL.... SRALTPSPVM GKASNNPPFV GKTTDKSPFV **PDDIGQSPIV** PDDICOSPIVSP.. GKASHTAPFV GAAAASA... EPPILYSE.. • • • • • • • • • PEDIGOAPIV TNNSSEQRV. TNSSADHRV. CQL...GKYT DOMVSALLDA SHWKORRKFL SHWKORRKFL SHWKOKPKFL CQL...GKYT GLNPS.... TKKKARSILT TKAKARAILT PLLVNPASLA PTLVS.... GGSGS.... NKVKARVILS TALVPQLSTI FSPCQDIQLI PPLIN..... VSHIEGYECQ PIFLN.... KNSLALSLTA KAHQETFPAL KAHQETFPSL ETYVE..ANH DOCVEGPGGT EAYLKNFN.H NAYLKNFN. H DSYIKSFP.L NAQCQVICTL IVPATLPQLT IAPAKEPSVN EAHRSTNAOG EAHRSTNAQG EAHVATNAOG . TEETTOKLT PSPLMIKRSK EEWDLIHVAT EEWDLIHIAT EVGELIEKVR QLEELITKVS EAELAVEPKT EAELAVEOKS DLKSLAKRIY DLKAFSKHIY DLRALAKHLY VAGLTSQLIT ETSENPGNKT ESQALSQRFT POSPEEGITY EEWELIKTUT minimal start site 725 SIGHKPEPTD EGSQYNPQVA AGDHRAANLW DIDQLNPESA TSAMSN ALPOPLGVPN dadada di OOO SLOCIPEPTP SLOGRPEPTP ECSESYTLTP GSPUSYELSP NEDMPVERIL PEEMPVDRIL EHD LEDSETA ..GVSQ TPI hVDR her hGR hPR **FAR** hPPARgamma rTRalpha hTRalpha hTRbeta hRARalpha hRARgamma hRXRalpha hRXRbeta hPPARalpha hPPARbeta

FIG.3M

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rTRalphaSMPDGDKVD LEAFSEFTKI ITPAITRVVD FAKKLPHFSE LPCEDQIILL hTRalphaSMPDGDKVD LEAFSEFTKI ITPAITRVVD FAKKLPHFSE LPCEDQIILL hTRbetaSLD IDLHDKFSEL STKCIIKTVE FAKKLPHFCE LPCEDQIILL hRARgamma
rTRalpha hTRalpha hRARalpha hRARgamma hRXRalpha hPPARalpha hPPARalpha hPPARalpha hPPARARalpha hPPARGamma hPPARGamma hPPARGamma

FIG.3N

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900		QLKNGGLGV VSDAIFELGK	•	NAGFGP LTDLVFAFAN	NAGFGP LIDLVFAFAG	S. AGVGAI FDRVLTELVS	WGAI FDRVLTELVS	SLRKPFCD IMEPKFDFAM	SLRKPFSD IIEPKFEFAV	SLRKPFGD FMEPKFEFAV	AI NLEEIREFAK	I FDMLLAT.SS	LPCHYD QCKHMLYVSS	ESSFYS LCLTHWQIPQ	QSAMYE LCQGMHQISL	OYSWHGLHVF AMGWRSFINV NSRMLYFAPD LVFNEYRHH KSRMYS QCVRHRHLSQ	
			•	NAGFGP	N. AGEGP	AGVGAI	VGAI	FCD	SD	g	H	H	۵	S	Œ	(S	
A 10 AGAIMA GOS TO TOTOGO GO CONTRACTO	VARAGER	QLK.	χ.		•	S	S.AGVGAI	SLRKE	SLRKPI	SLRKPF			LPCHY	ESSFY	QSAM	KSRM	
	Ē	HAVKRE	HAVIRGOL	LTLNRTQMH.	LILNRIQMH.	LHVHRNSAH.	LHVHRNSAH.	F. ITREFLK.	F.VTREFLR.	F. MTREFLK.	HPTVGQLVNK	LLLDRNQGK.	LIINEQRMT.	LILNEQRMK.	LVFNEEKHH.	LVFNEYRHH.	
	ESDILITSCE	ESDILILSGE	ESETLTLNGE	EQDIMIFSDG	EQDIMIFSDG	RAGWNELLIA SFSHRSIA VXDGILLATG LHVHRNSAH.	RAGMNELLIA SFSHRSID VRDGILLATG LHVHRNSAH.	KYGUYEAIFA HLSSUMNK DGHLVAYGNG F.ITREFLK.	MLASIVNK DGLLVANGSG F.VTREFLR.	KYGVHEIIYT MLASLMNK DGVLISEGQG F.HTREFLK.	APSKVIIAPO PSVVKPVTSL TAAGVIACGE HPTVGQLVNK	GLVWRSME HPGKLLFAPN LLLDRNQGK.	ALGWRSYRQS SANLLCFAPD LIINEQRHT.	SGOMLYFAPD LILNEORMK.	NSQFLYFAPD LVFNEEKHH.	NSRMLYFAPD	
	RAAVRYDP	RAAVRYDP	RAAVRYDP	RICTRY TP	RICTRYTP	SFSHRSIA	SFSHRSID	HLSSVHNK	MLASIVNK	HLASLMNK	PSVVKPVTSL	GLVWRSHE	ALGWRSYROS	GLGWRSYKHV	OYSWHCLSSF ALSWRSYKHT	AMGWRSFTNV	
841	KGCCHEIMSL	KGCCHEIHSL RAAVRY DP ESDILILSGE HAVKREQLK.	KGCCHEIMSL RAAVRY DP ESETLTLNGE MAVIRGOLK	KAACLDILIL RICTRY TP EQDIMIFSDG LILNRIQMH	KAACLDILML RICTRYTP EQDIMIFSDG LILNRIQMH	RAGWNELLIA	RAGWNELLIA	KYGUYEAIFA	KYGVHEAIFA	KYGVHEIIYT	APSKVIIAPO	ECAMLEILMI	OXSWMFLMAF	OYSWMSLHVF	OYSWMCLSSF	QY SWHGLHVF	•
,	rTRalpha	hTRalpha	hTRbeta	hRARalpha	hRARdamma	hRXRalpha	hRXRbeta	hppagalnha	hpparbeta	PODE BURNES	HVDR	her	มีเล	hPR	P. P	har har	

FIG.30

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. FEHYV LA...FEHYV LA...FEHYI EA...LKVYV EA...LRLYA

.. RSGLLCVD KIEKSQEAYL .. RSGLLCVD KIEKSQEAYL

MSTD....

EVALLQAVIL EVALLQAVLL EVALLQAVLL ETGILSAICL ETGLLSAICL ELGCLRAIVL

SLSAFNLDDT

rTRalpha hTRalpha

901

SLSAFNLDDT SLSSFNLDDT

HSTD. MSSD.

RIEKYQDSFL RVDMLQEPLL KVDKLOEPLL EVEALREKVY EVEVLREKVY

.. RPGLACVE

.. RQDLEQPD

ICGD.... ICGD

QLLPLEMDDA QLLPLEMDDT

hRARa 1 pha

hTRbeta

.. RHDLEEPE ... KGLSNPA ... KGLSNPS

FNPDS....

FNPDA.... cccb.... LCGD

ELGCLRAIIL

KHRDMQMDKT KMRDMRMDKT

hRXRa lpha hRXRbeta hPPARalpha

hRARgamma

IPVDGLKNOK FFDELRMNYI SAICRFEKLD STLKSLEEKD VPKDGLKSQE IPKDGLKSQA IPLEGLRSQT LNT LST TATEGPAYSQ LNSGVYTFLS LSS..... FSI

KELRKHVTKC

AFEEMRTNYI

KELDRIIACK

DTLIHLMAKA KELGKAIVKR

ITPKSAQKLK

PIEDIQDNLL

.. RPGLMNVP .. RPGLLNVK

LSGD

KFNALELDDS

KFNALELDDS

hPPARbeta

hPPARgamma

NFKIRRLSLG RFRHMNLOGE

hvdr her hGR hPR FHA

DLALFIAAII DLAIFIAVII LTQTQVGQAL

DISLEVAAII

KFNALELDDS

EFVCLKSIIL EXLCHKTLLL EFLCHKVLLL EYTIMKVLLL EFLCHKALLL

ELHRLQVSYE

OFVRLQLTFE

EFGWLQITPQ

EFVKLQVSQE

HIHRVLDKIT

LFDEIRHTYI **OFEEMRSSYI**

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AS...LEAYC

AS...LETYC HV...LRLHL RA...LEFHL QA...LELQL PVLERWLAEA

> HIEKMQEGIV RVEAIQDTIL

.. RPGLLNVG

CHASREL..H MKVEC..PTE LFPPLFLEVF

LFPPLFLEVF LLPPLFLEVF

CHASRFL..H MKVEC..PTE CHASRFL..H MKVEC..PTE

KVTDLRMIGA KVTDLRMIGA KITDLRSISA

WPKLL...H

FPKML...H FPRHL...H FAKLL...L FAKLL...L FPKLL...Q

AKRRPSRPHM RRRPSQPYH KHKYPEQPGR KOKY PEQQGR

KVTDLRMIGA

WPKLL...H WPKLL...H

NHRKHNIPHF NHRKHNIPHF NYRKHHVTHF

rTRalpha hTRalpha hTRbeta hRARalpha **hRARgamma** hRXRalpha

961

M. PPLIQEML M. PPLIREML

LKMEI..PGS

KGAERVI..T KGAERAI..T EHAQHMQ..R IKKTE..TET EHVQLLH..V IKKTE..TDM ILSHIRHMSN KGMEHLY..S QLHLYCLNTF RKNPTSCSRR FYQLT....K LLDSVQPIAR ELHQFTFDLL PQAIEVLNTY NLLNYCFOTF DLLEFCFYTF LLDSMHEVVE FYQLT...K LLDSMHDLVS KHTDLRQIVT KKRKRRTSFT LLDNLHDLVK KHADLRQLVT

FYQLT...K FYQLT....K

EGNSSQNWQR QKGVVSSSQR PNNSGOSWOR

EFPAMLVEII

DFPEMMAEII

IKSHM..VSV

EFPEHMSEVI

IQSRA..LSV

RESHA..LKV

EITEIAKELN

FEKNSLPTGQ MKC. K.. NVV LD.KT..HSI

LHEFVGGEPS

KLNHPESSQL ELWNOKGOON GLTLQQQHQR

> hvdr her hGR hPR **h**HR

LAQLL...L

FPKLL...Q FAKVL...Q

QSNHPDDIFL QANHPDAQYL PLYDLLLEML EFPEMLAEII

SLHPLLQEIY

SCHPLLQEIY

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hRXRbeta hPPARalpha hPPARbeta hPPARgamma

18/50

FKL. I.. GDT IKKTE..SDA

KCLEHLF..F

EHAQLVQ..I

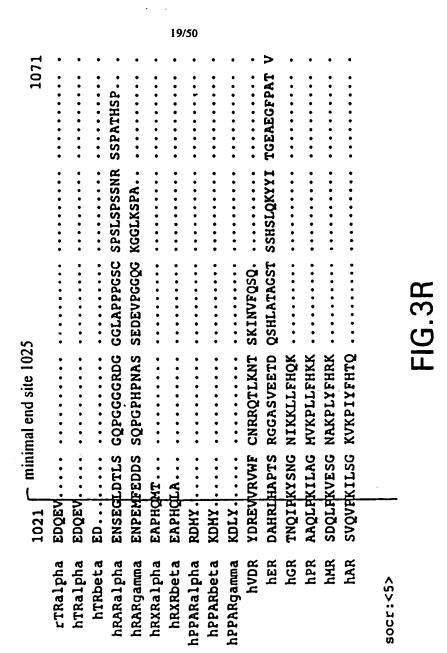
PIDTFLMEML PIDTFLHEM ALHPLLQEIY

FKL. I. . CDT

KCLEHLF..F

KITDLRGIST RLPALRSIGL RLPALRSIGL KHADLROLVT

LKMEI..PGP



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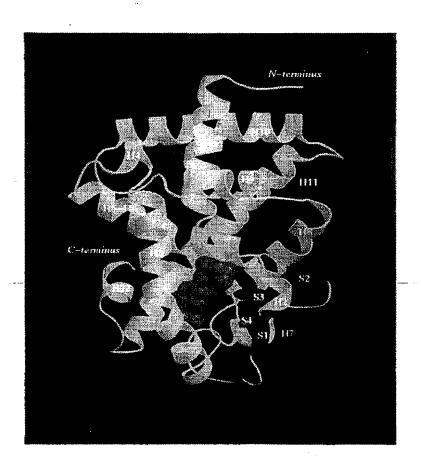
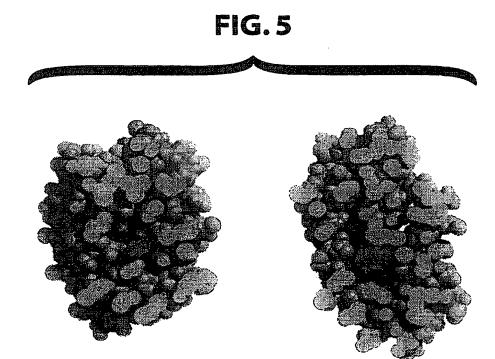


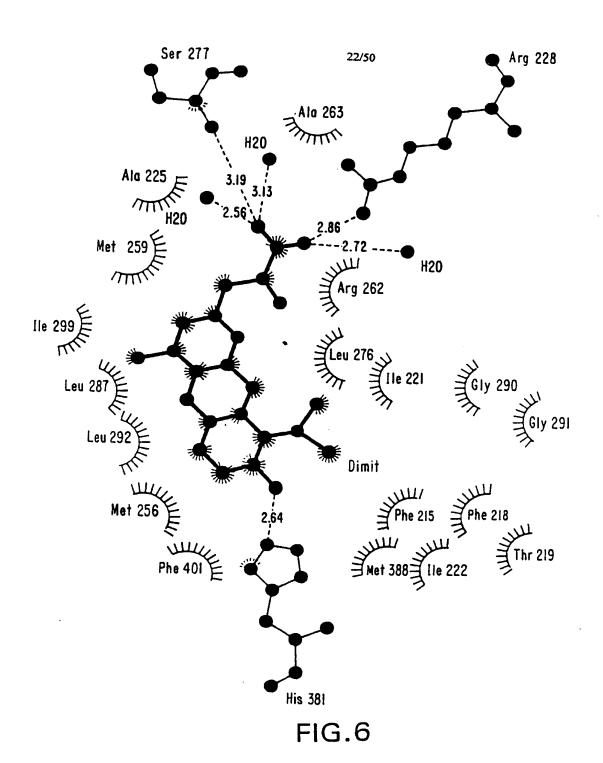
FIG. 4

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FIG. 7

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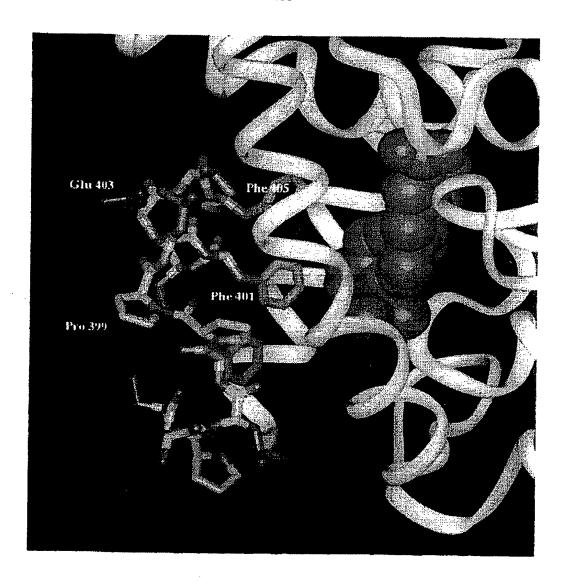


FIG.8

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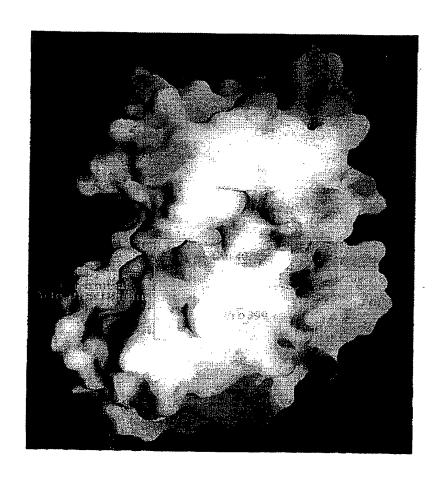


FIG. 9

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AGONISTS

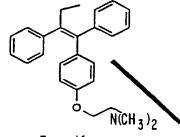
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ANTAGONISTS

Retinoic Acid

(CH₂)₁₀ CON(CH₃)(CH₂)₃CH₃

Estradiol



Diethylstilbestrol

Progesterone

FIG.10

shows position of extension group

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Compound	RCOX
TSI	Ph ₂ CHCO ₂ NHS
TS2	C ₁₆ H ₃₃ CO ₂ NHS
TS3 ·	FMOC-CI
TS4	tB 0C ₂ 0
TS5	tB0C20

FIG.11

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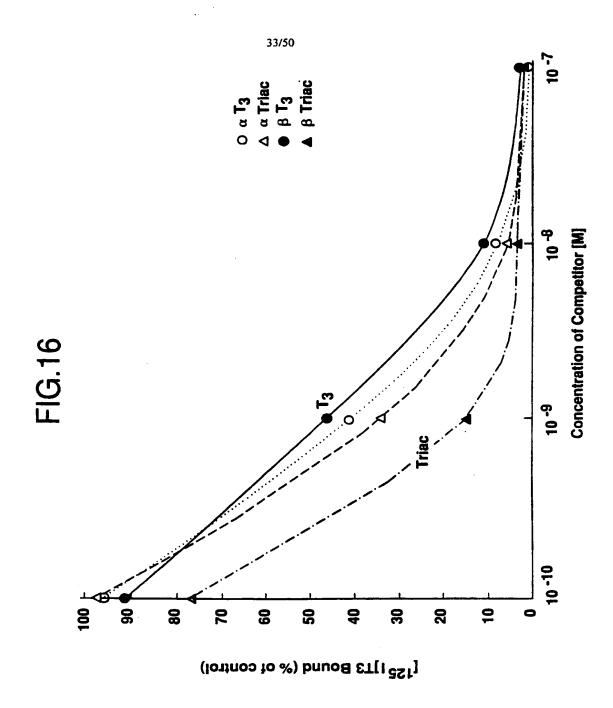
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$$\begin{array}{c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

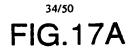
FIG.15

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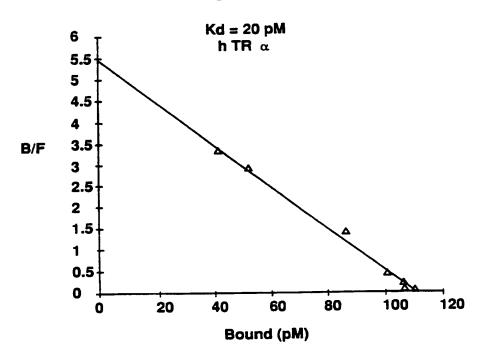
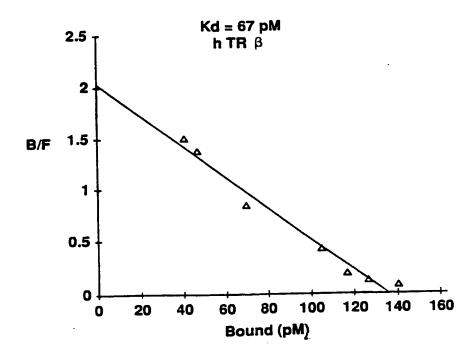
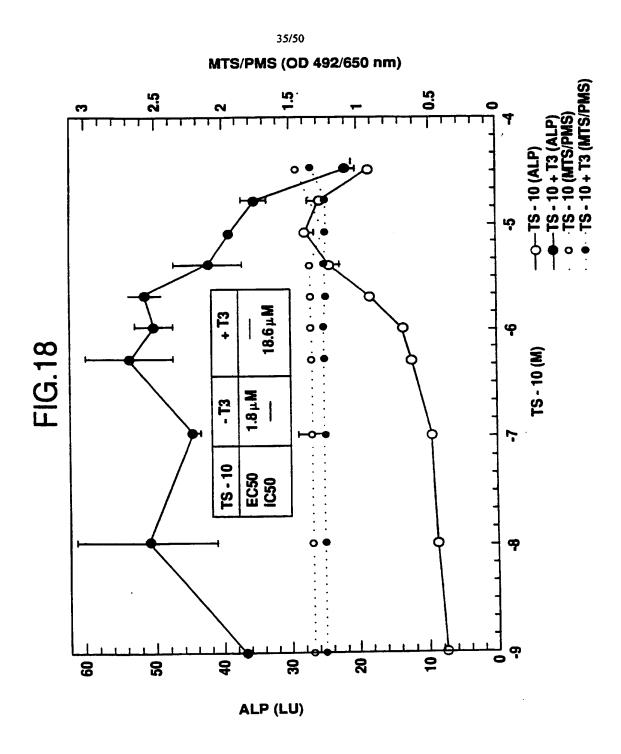


FIG.17B

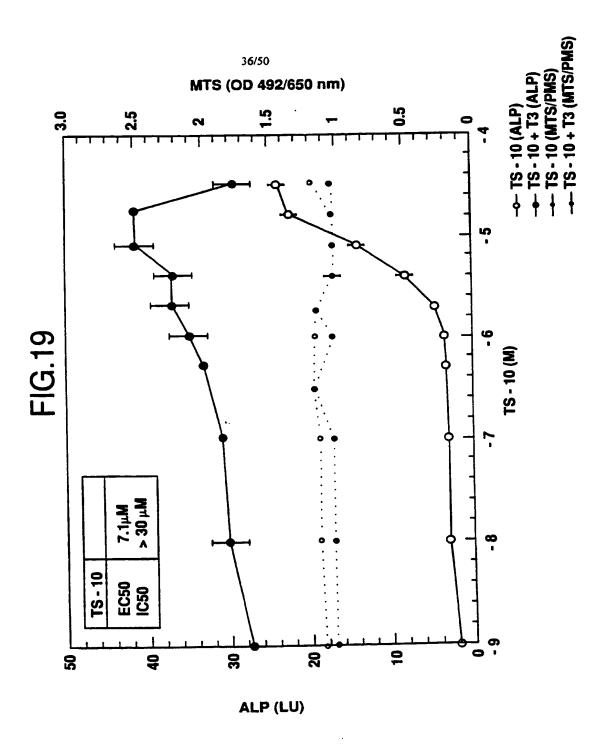


SUBSTITUTE SHEET (RULE 26)

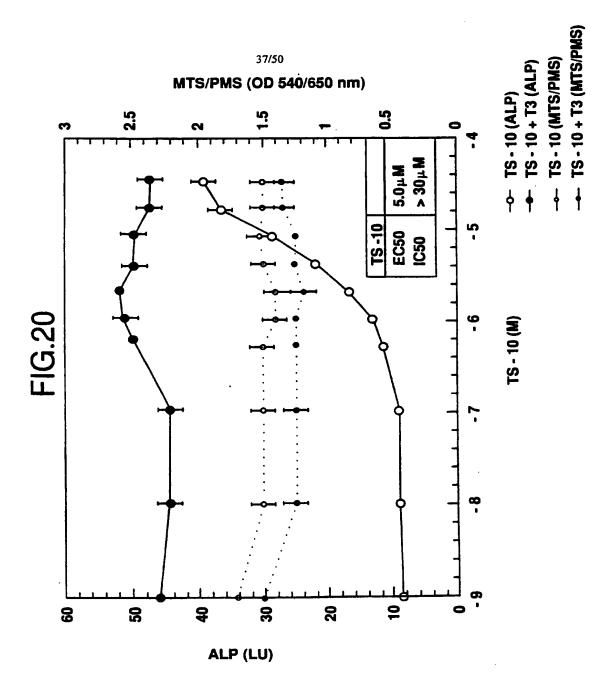
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SUBSTITUTE SHEET (RULE 26)



SUBSTITUTE SHEET (RULE 26)



SUBSTITUTE SHEET (RULE 26)

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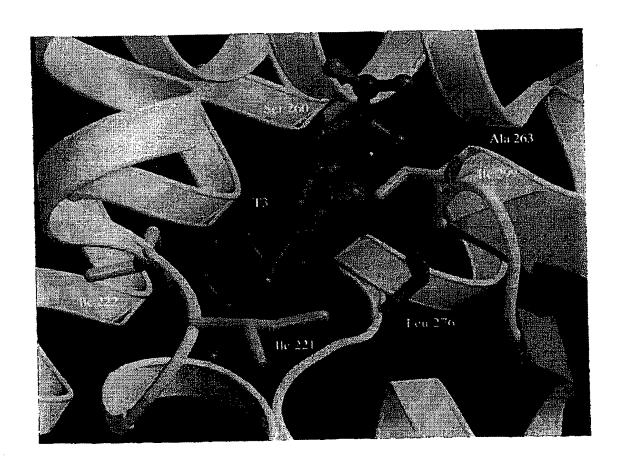


FIG. 21

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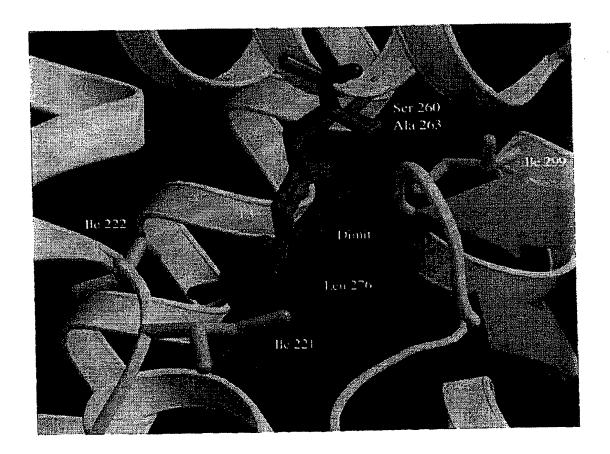


FIG. 22

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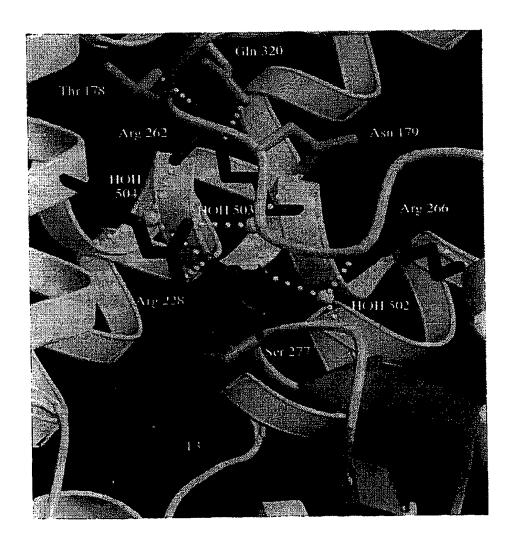


FIG. 23

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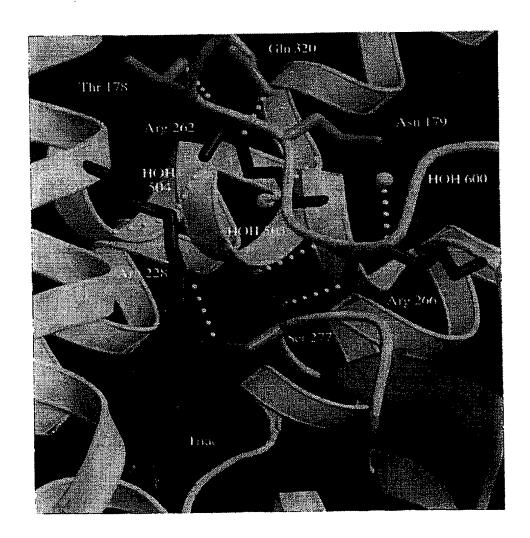


FIG. 24

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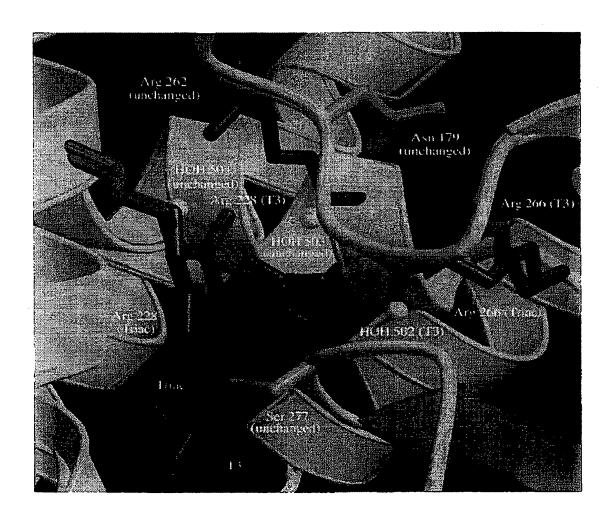


FIG. 25

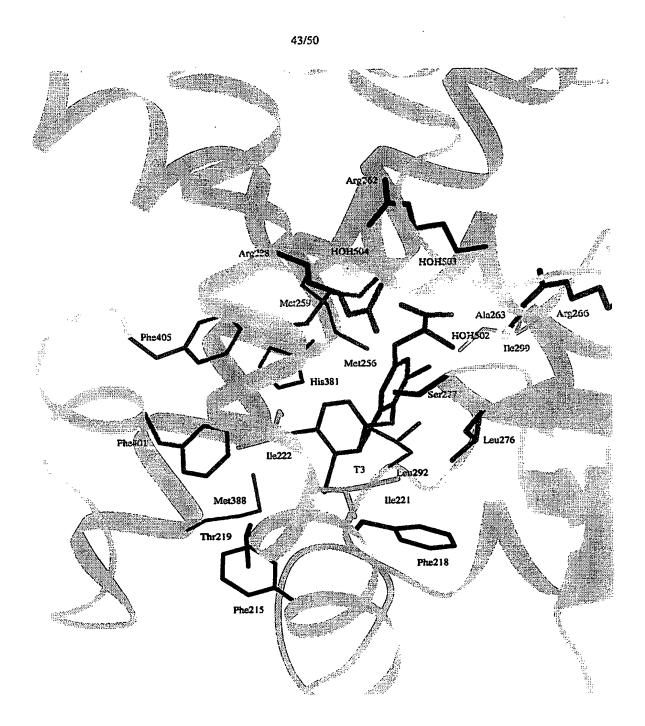


FIG. 26A

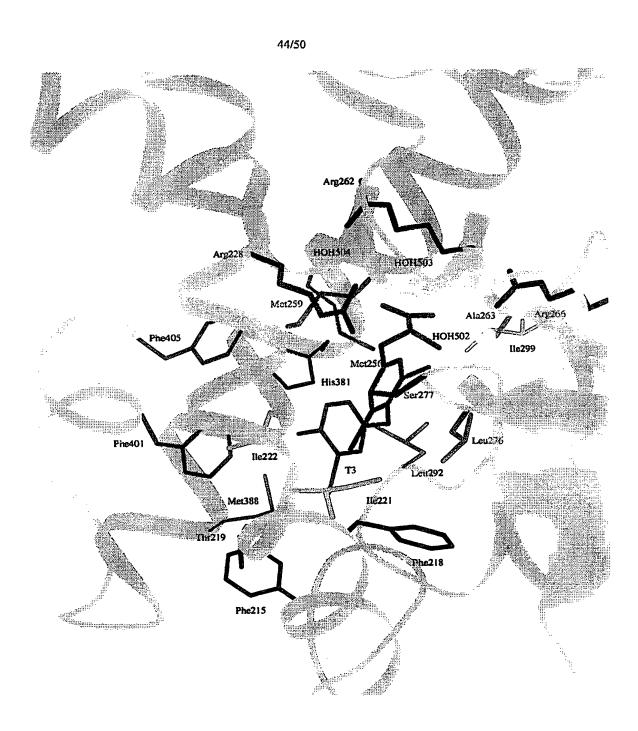


FIG. 26B

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Thyroid Hormone Receptor Beta with GC1

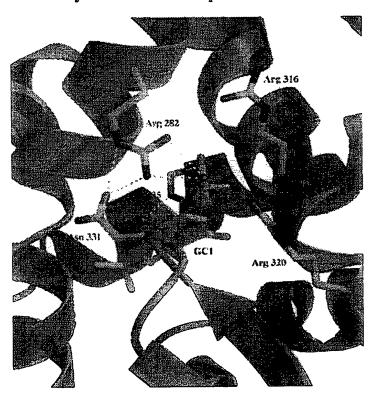


FIG. 27

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Thyroid Hormone Receptor Beta with Triac

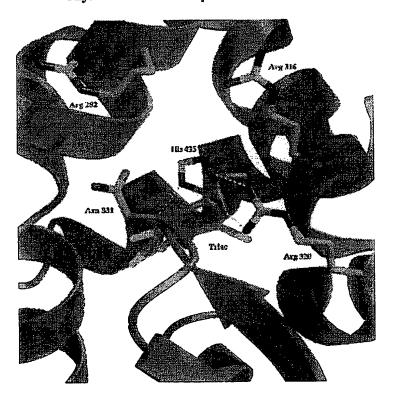


FIG. 28

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Structural Differences Between TR-b with GC1 and TR-a with Dimit



FIG. 29

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Structural Differences between TR LBD isoforms with Triac

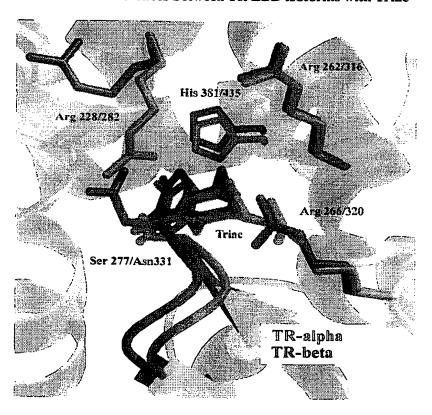
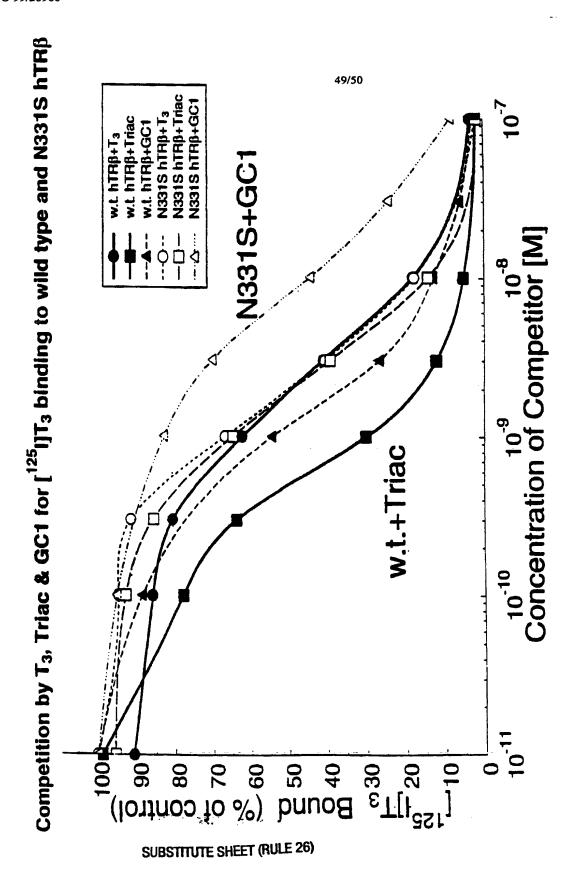


FIG. 30

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Atomic Numbering for Thyronine-like Ligands

Ligand	R1	R3	R5	X	R3'	R4'
Dimit	amino propionic	C19	C20	02	iPr	01
IpBr,	amino propionic	BR1	BR2	02	iPr	O 1
Ť,	amino propionic	I1	13	02	12	O 1
Triac	acetic acid	I1	13	02	12	01
GC1	oxyacetic acid	C19	C20	C21	iPr	O 1

FIG.32

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